Where Deep Learning Losses Come From

Likelihood, cross-entropy, and regularization from probability

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ES 667 · Deep Learning · IIT Gandhinagar

Three familiar losses, one probabilistic origin

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Objective. Derive each term from an explicit likelihood or prior.

Outline

1. **Predictive distributions** — what the network says about Y given x
2. **Likelihood** — how observed data score candidate parameters
3. **Negative log-likelihood** — why products become trainable sums
4. **Output losses** — Gaussian $\rightarrow$ MSE; Bernoulli/categorical $\rightarrow$ cross-entropy
5. **Priors and MAP** — why regularizers belong in the same objective

Probability primer

Discrete distributions assign probability to outcomes

V VISUAL

The **support** $\mathcal{S}_Y$ is the set of values that Y can take.

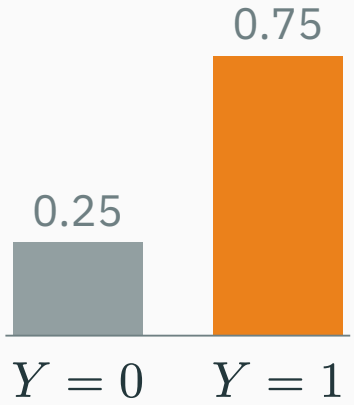
Probability mass function (PMF)

$$p_{Y(y)} = P(Y = y), \quad y \in \mathcal{S}_Y$$

$$p_{Y(y)} \geq 0, \quad \sum_{y \in \mathcal{S}_Y} p_{Y(y)} = 1$$

Examples. Bernoulli: $\{0, 1\}$ · categorical: $\{1, ..., K\}$ · Poisson: $\{0, 1, 2, ...\}$

Bernoulli(0.75) **PMF**



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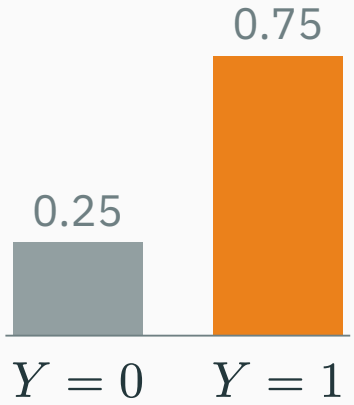

each bar is an outcome probability

Exact values can have nonzero probability: here $P(Y = 1) = 0.75$.

Continuous distributions assign density across a support

V VISUAL

The **support** may be bounded or unbounded:

$\mathcal{S}_Y = [a, b]$

for a Uniform variable; $\mathcal{S}_Y = \mathbb{R}$ for a Gaussian.

Probability density function (PDF)

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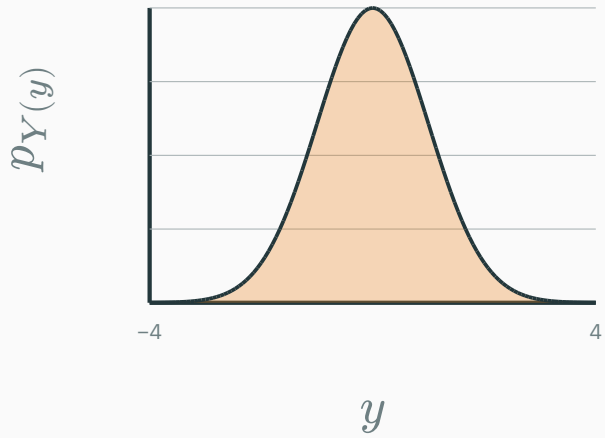

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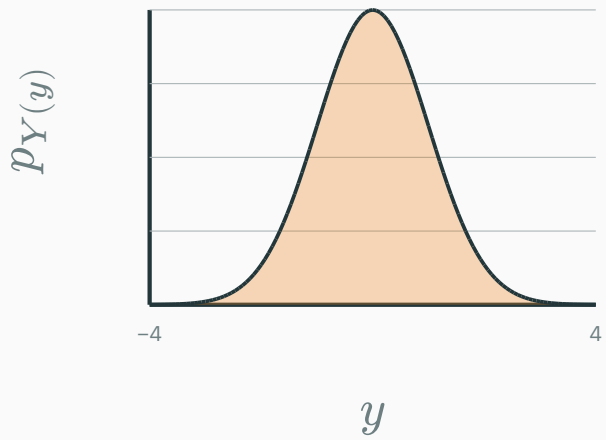

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For continuous Y, probability comes from area under the density.

Density is not probability

V VISUAL

For a continuous Y, probability comes from **area**:

$$P(a \leq Y \leq b) = \int_a^b p_{Y(y)} \, \mathrm{d}y$$

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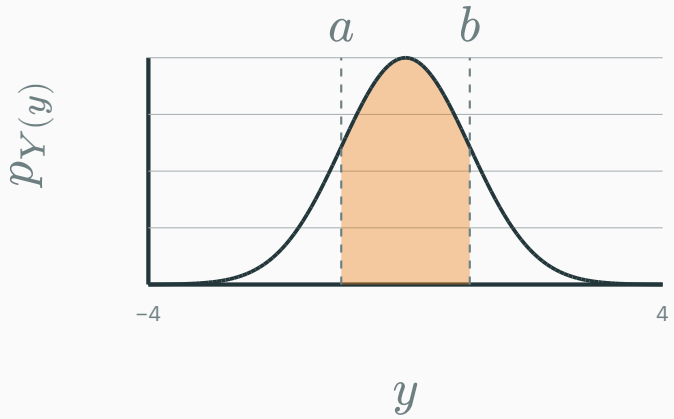
For a continuous Y, probability comes from **area**:

$$P(a \leq Y \leq b) = \int_a^b p_{Y(y)} \, \mathrm{d}y$$

$p_{Y(y)} \neq P(Y = y)$ — a density can **exceed 1**; only *integrals* are probabilities.



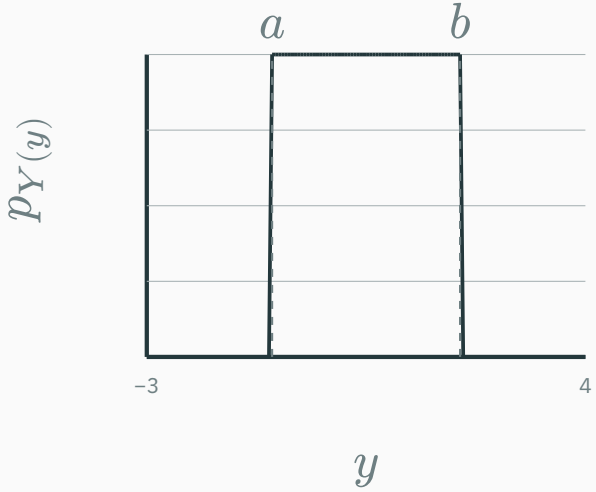
the shaded area is $P(a \leq Y \leq b)$

Uniform distribution: support matters

V VISUAL

$$Y \sim \mathcal{U}(a,b) \quad p_{Y(y)} = \begin{cases} 1/(b-a) & a \le y \le b \\ 0 & \text{otherwise} \end{cases}$$

The support matters: outside $[a,b]$, the density is exactly 0.



Gaussian distribution

V VISUAL

$$Y \sim \mathcal{N}(\mu, \sigma^2) \qquad p(y) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right)$$

μ is the mean; $\sigma > 0$ is the standard deviation (scale); σ^2 is the variance.

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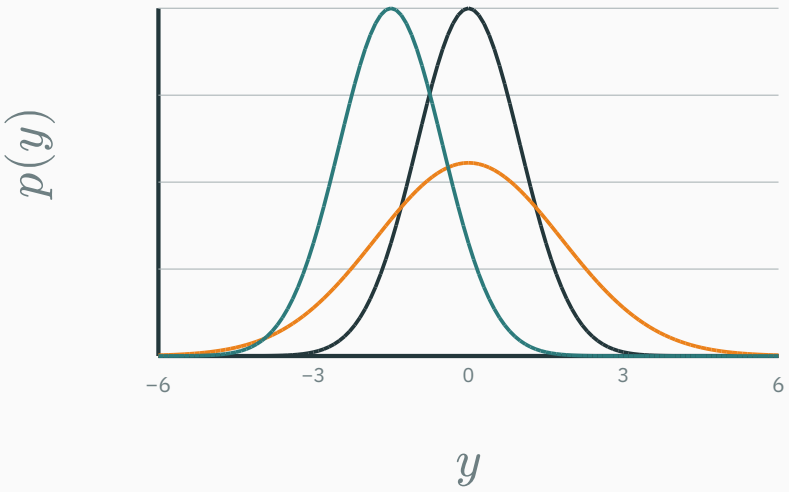
$\mu = 0, \sigma = 1$ $\mu = 0, \sigma = 1.8$ $\mu = -1.5, \sigma = 1$



Only two knobs: **location** μ and **scale** σ.

From probability to likelihood

Read the model notation one symbol at a time

Q QUESTION

$$p_{\boldsymbol{\theta}}(y \mid \boldsymbol{x})$$

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$\boldsymbol{X}$ / $\boldsymbol{x}$	$\boldsymbol{X}$ is the random input vector; $\boldsymbol{x}$ is one observed input
Y / y	Y is the random target; y is one possible or observed value
$\boldsymbol{\theta}$	the **parameter vector** — the model's learned weights and biases
$p_{\boldsymbol{\theta}}(y \mid \boldsymbol{x})$	the probability (discrete Y) or density (continuous Y) assigned to y, **given** $\boldsymbol{x}$

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Read aloud: "model θ's probability or density for y, given x."

A point prediction summarizes a distribution

V VISUAL

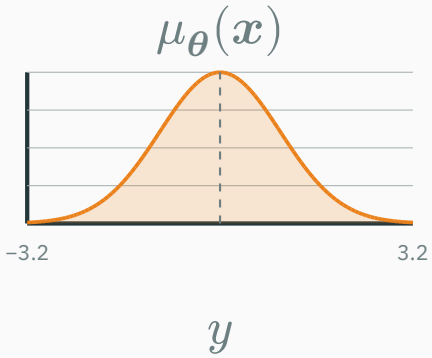
REGRESSION · $Y \in \mathbb{R}$

Point prediction: mean of $Y \mid \boldsymbol{X} = \boldsymbol{x}$

$$\hat{y}(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{\theta}}[Y \mid \boldsymbol{X} = \boldsymbol{x}] = \mu_{\boldsymbol{\theta}}(\boldsymbol{x})$$

Full predictive distribution

$$Y \mid \boldsymbol{X} = \boldsymbol{x} \sim \mathcal{N}\big(\mu_{\boldsymbol{\theta}}(\boldsymbol{x}), \sigma^2_{\boldsymbol{\theta}}(\boldsymbol{x})\big)$$



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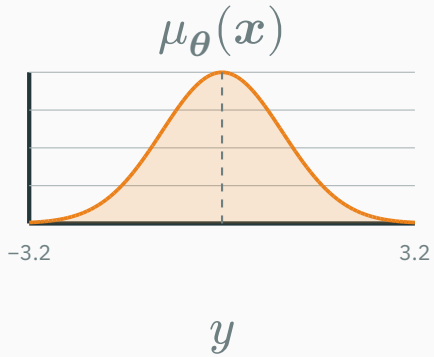


BINARY CLASSIFICATION · $Y \in \{0, 1\}$

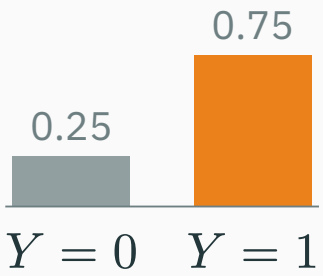
Point prediction: most probable outcome (mode)

$$\hat{y}(\boldsymbol{x}) = \mathbf{1}[p_{\boldsymbol{\theta}}(\boldsymbol{x}) \geq 0.5]$$

Full predictive distribution

$$Y \mid \boldsymbol{X} = \boldsymbol{x} \sim \text{Bernoulli}(p_{\boldsymbol{\theta}}(\boldsymbol{x}))$$

example: $p_{\boldsymbol{\theta}}(\boldsymbol{x}) = 0.75$



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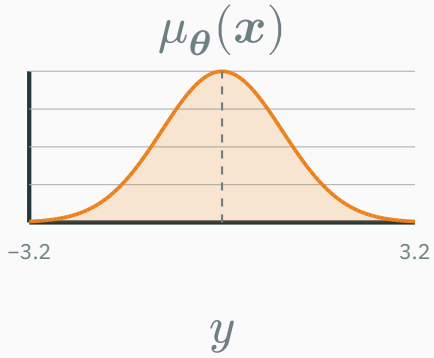

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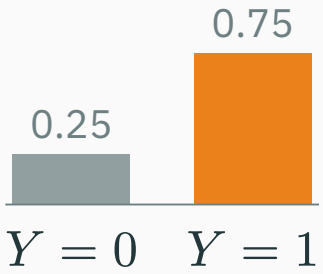

Neural network: $x \to$ distribution parameters. Prediction: $\hat{y}$ = mean or mode.

Prediction fixes the model and varies the outcome

V VISUAL

Example: $Y \in \{0, 1\}$. Fix the input $x^\star$ and one parameter setting θ_A.

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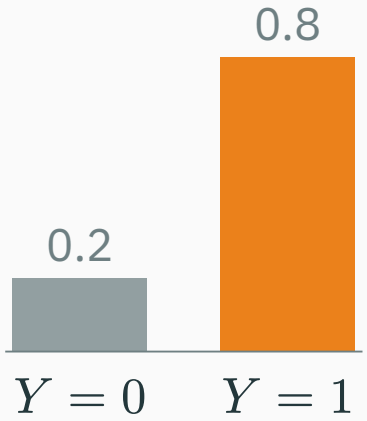
$$p_{\theta_A}(Y = 0 \mid x^\star) = 0.20$$

$$p_{\theta_A}(Y = 1 \mid x^\star) = 0.80$$

$$0.20 + 0.80 = 1$$

We vary the possible value of Y while keeping θ_A and $x^\star$ fixed.

predictive distribution



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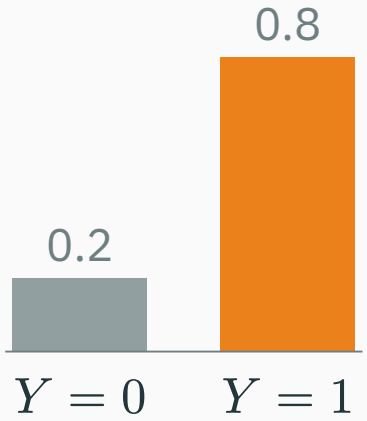

$$\hat{y}(x^\star) = \arg\max_y p_{\theta_A}(y \mid x^\star) = 1$$

One observed label gives one likelihood score

D DERIVATION

Now observe $y^\star = 1$ for the input $\boldsymbol{x}^\star$, so $\mathcal{D} = \{(\boldsymbol{x}^\star, 1)\}$.

$$L(\boldsymbol{\theta}; \mathcal{D}) = p_{\boldsymbol{\theta}}(y^\star = 1 \mid \boldsymbol{x}^\star)$$

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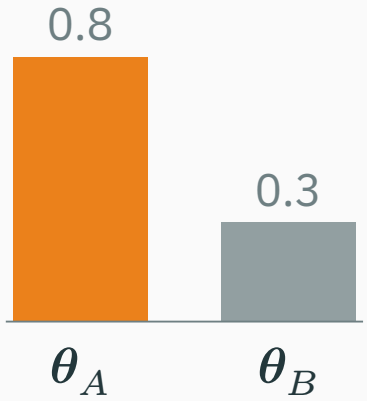
Candidate A: $L(\theta_A; \mathcal{D}) = 0.80$
Candidate B: $L(\theta_B; \mathcal{D}) = 0.30$

$$L(\theta_A; \mathcal{D}) > L(\theta_B; \mathcal{D})$$

θ_A makes the observed label $y^\star = 1$ less surprising.

likelihood of the fixed observation



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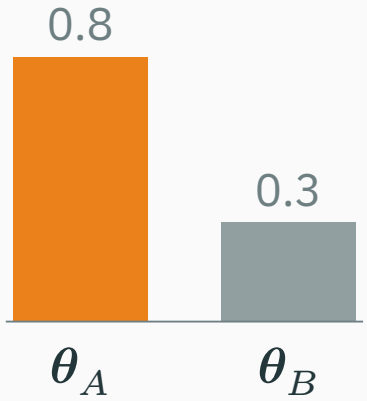

Likelihood is a **score as a function of θ**; the scores need not sum to 1 over parameter settings.

One continuous observation gives a likelihood too

D DERIVATION

Suppose $Y \mid \mu \sim \mathcal{N}(\mu, 1)$ and we observe the fixed value $y^\star = 1$.

$$L(\mu; y^\star = 1) = \left[p_{Y(y \mid \mu)}\right]_{y=1} = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(1-\mu)^2}{2}\right).$$

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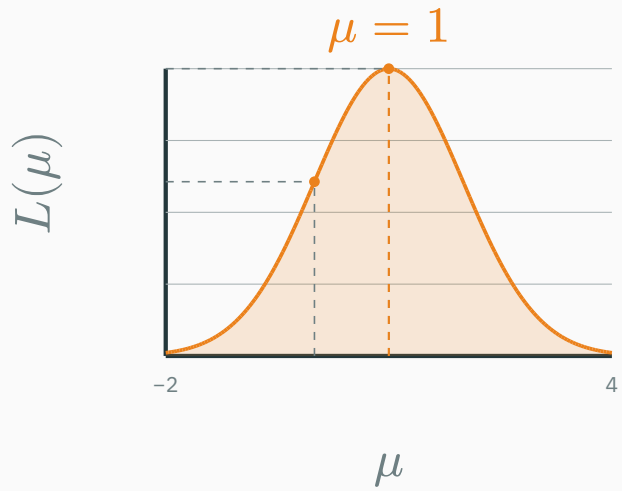
Candidate $\mu = 1$: $L(1) \approx 0.399$
Candidate $\mu = 0$: $L(0) \approx 0.242$

$\mu = 1$ centres the Gaussian at $y^\star = 1$ and gives the largest **density**.



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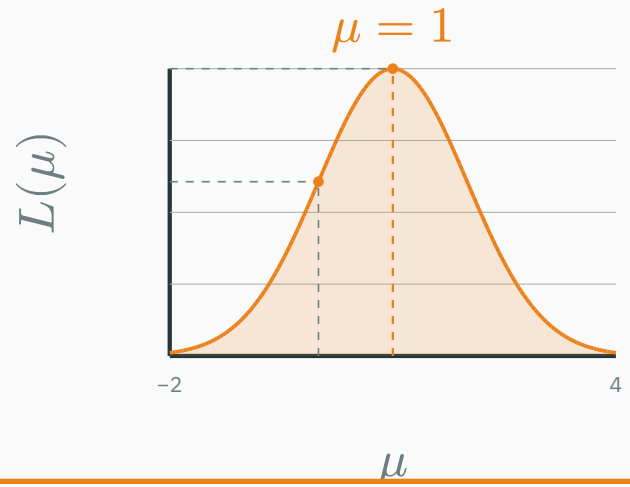

For continuous Y, this is a density value—not $P(Y = 1)$. Fix the observation, then compare parameter values.

A dataset needs a joint likelihood

Q QUESTION

For two observations, the likelihood starts as a **joint** probability or density:

$$L(\boldsymbol{\theta}; \mathcal{D}) = p_{\boldsymbol{\theta}}(y_1, y_2 \mid \boldsymbol{x}_1, \boldsymbol{x}_2).$$

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We may write a product only after making an assumption about how the observations relate.

Question: when is $p(y_1, y_2 \mid \boldsymbol{\theta}) = p(y_1 \mid \boldsymbol{\theta}) p(y_2 \mid \boldsymbol{\theta})$ valid?

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The product is a consequence of **conditional independence**; it is not automatic.

Independent means “no extra information”

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Independence is what licenses multiplication.

Identically distributed means “the same sampling rule”

D DERIVATION

Coin flips

$Y_i \mid \theta \sim \text{Bernoulli}(\theta)$ for every i.
Each flip uses the same bias θ.

Supervised learning

The pairs $(\boldsymbol{X}_i, Y_i)$ come from the same population, and one shared $\boldsymbol{\theta}$ defines $p_{\boldsymbol{\theta}}(y_i \mid \boldsymbol{x}_i)$.

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i.i.d. = independent observations + one common data-generating rule.

Independence and identical distribution can fail separately

D DERIVATION

Not independent: daily weather

Tomorrow's weather depends on today's. A first-order Markov model writes

$$p(y_{1:T} \mid \theta) = p(y_1 \mid \theta) \prod_{t=2}^{T} p(y_t \mid y_{t-1}, \theta).$$

The factors are **conditional on the previous day**, not independent marginals.

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$$p(y_{1:T} \mid \theta) = p(y_1 \mid \theta) \prod_{t=2}^{T} p(y_t \mid y_{t-1}, \theta).$$

The factors are **conditional on the previous day**, not independent marginals.

Independent but not identical: two sensors

Two sensors measure the same temperature μ independently, but have different noise levels:

$$Y_i \mid \mu \sim \mathcal{N}(\mu, \sigma_i^2), \quad \sigma_1 \neq \sigma_2.$$

The likelihood is a product, but its factors use different σ_i.

Independence and identical distribution can fail separately

D DERIVATION

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i.i.d. is a useful special case—not a universal law.

Worked example: dependence changes the product

D DERIVATION

Let R_1 mean “rain today” and R_2 mean “rain tomorrow”. Suppose

$$P(R_1) = 0.4, \quad P(R_2|R_1) = 0.8, \quad P(R_2|\neg R_1) = 0.2.$$

1. Use the conditional rule

$$\begin{aligned} P(R_1, R_2) &= P(R_1)P(R_2|R_1) \\ &= 0.4 \times 0.8 = 0.32. \end{aligned}$$

Both days are rainy with probability 0.32.

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$$P(R_2) = 0.4 \times 0.8 + 0.6 \times 0.2 = 0.44.$$

If the days were independent,

$$P(R_1)P(R_2) = 0.4 \times 0.44 = 0.176,$$

not 0.32.

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Dependence does not forbid multiplication: use a conditional probability.

Worked example: independent does not mean identical

D DERIVATION

Given smoke S, two alarms act independently, but their sensitivities differ:

$$P(A_1 = 1|S) = 0.9, \quad P(A_2 = 1|S) = 0.6.$$

Independence

Both alarms ring with probability

$$P(A_1 = 1, A_2 = 1|S) = 0.9 \times 0.6 = 0.54.$$

The product is valid.

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Alarm 1 detects smoke 90% of the time; Alarm 2 detects it 60% of the time.

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We cannot reuse one common factor for both alarms.

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Independent says “multiply”; identical says “reuse the same sampling rule”.

IID turns the joint likelihood into per-example factors

D DERIVATION

For i.i.d. supervised examples, treat the observed inputs as fixed. Conditional independence gives

$$p(\mathcal{D} \mid \boldsymbol{\theta}) = \prod_{i=1}^{n} p_{\boldsymbol{\theta}}(y_i \mid \boldsymbol{x}_i).$$

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Next we compute this product, then introduce a transform that makes it easier to optimize.

This is the bridge from one-example likelihood to a dataset loss.

Work two tiny Bernoulli datasets

D DERIVATION

Compare a fair coin $\theta = 0.5$ with a head-biased coin $\theta = 0.8$.

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Observed data	$L(0.5)$	$L(0.8)$	**Which explains it better?**
H, T	$0.5(0.5) = 0.25$	$0.8(0.2) = 0.16$	fair coin
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Multiply one Bernoulli term per independent flip.

Two Gaussian measurements: multiply densities

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Candidate $\mu = 1.5$

$p(y_1|\mu) \approx 0.352$

$p(y_2|\mu) \approx 0.352$

$L(1.5) \approx 0.352 \times 0.352 = 0.124$

Candidate $\mu = 0$

$p(y_1|\mu) \approx 0.242$

$p(y_2|\mu) \approx 0.054$

$L(0) \approx 0.242 \times 0.054 = 0.013$

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For continuous data we multiply densities; $\mu = 1.5$ gives the larger likelihood.

Maximum likelihood estimation

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Maximum likelihood estimation (MLE). Choose the parameter values that assign the highest likelihood to the observed dataset.

Companion notebook: distributions, MLE, and MAP in PyTorch

I INTERACTIVE

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↗ colab.research.google.com/github/nipunbatra/dl-teaching/blob/master/notebooks/L01/00_likelihood_iid_worked_examples.ipynb

Explore `torch.distributions`, `log_prob`, sampling, i.i.d. factorization, coin-toss MLE, Gaussian regression, Bernoulli classification, and MAP with Gaussian, Laplace, and Student-t priors.

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Short companion: fit the same line with Gaussian/MSE, Laplace/MAE, and Student-t losses; then see which observations control each estimate.

Coin flips: a likelihood you can compute

D DERIVATION

Observed: $H, H, T, T, T, H, H, T, T, T$

Hence $n_H = 4$ and $n_T = 6$.

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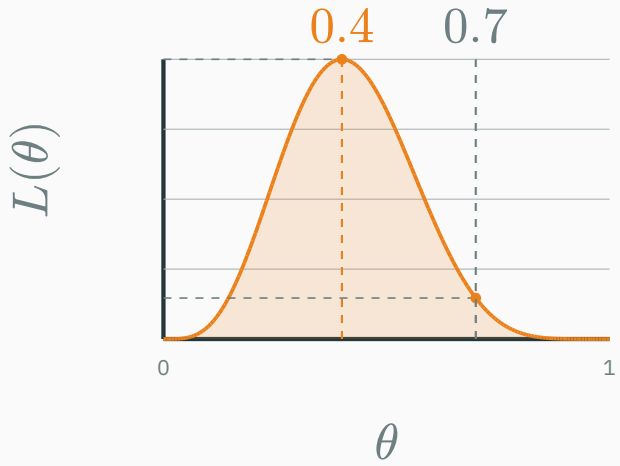
Because the flips are i.i.d.,

$$L(\theta) = \prod_i p(x_i \mid \theta)$$

$$= \theta^{n_H}(1-\theta)^{n_T}$$

$$= \theta^4(1-\theta)^6$$



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$$L(0.7) \approx 0.000175$$

about $6.8\times$ larger at $\theta = 0.4$

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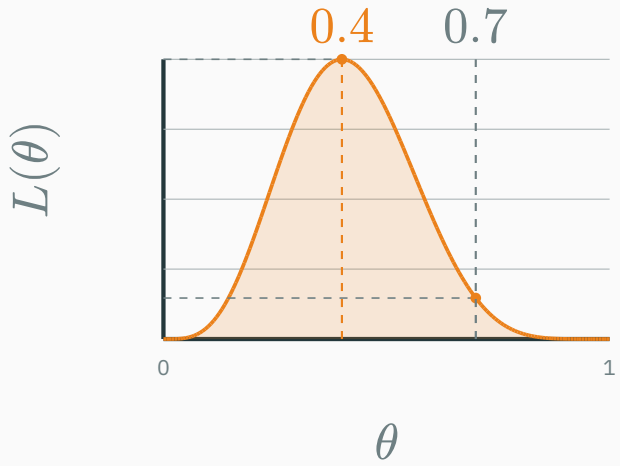

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The likelihood peaks at $\theta = 0.4$ — the observed head fraction $\frac{4}{10}$.

Coin flips: calculate the log-likelihood

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The **log-likelihood** is the logarithm of the likelihood — not a different model:

$$\ell(\theta) := \log L(\theta) = \log\left[\theta^4(1-\theta)^6\right] = 4\log\theta + 6\log(1-\theta)$$

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Likelihoods below 1 have negative logs; among them, -6.73 is the larger value.

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The observed sequence has higher log-likelihood at $\theta = 0.4$.

Why logs? The maximizing parameter does not change

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The logarithm is **strictly increasing** on positive numbers:

$$a > b > 0 \quad \Longrightarrow \quad \log a > \log b$$

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apply the increasing function $\log$

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Both likelihood and log-likelihood rank $\theta = 0.4$ above $\theta = 0.7$.

Poisson example: logging preserves the peak

V VISUAL

Suppose $Y \sim \text{Poisson}(\lambda)$ and the observed count is $y = 3$.

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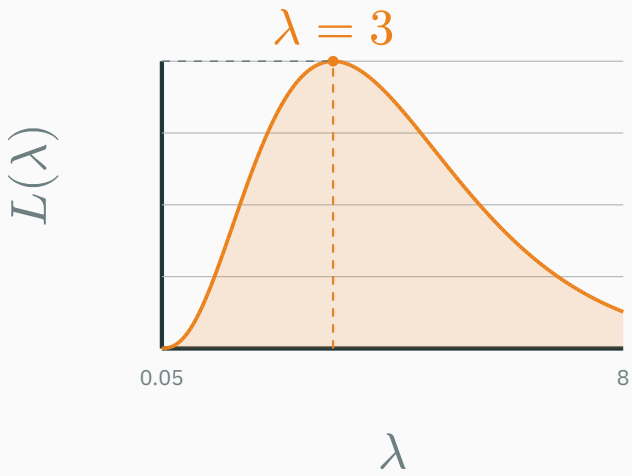
LIKELIHOOD

$$L(\lambda) = e^{-\lambda}\frac{\lambda^3}{3!}$$



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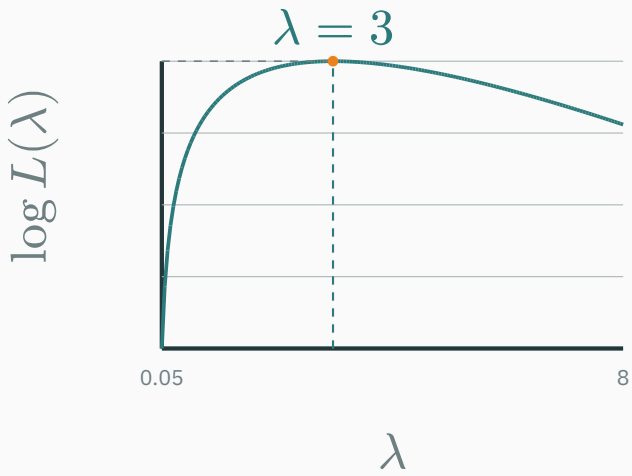
$$\log L(\lambda) = 3\log\lambda - \lambda - \log 3!$$



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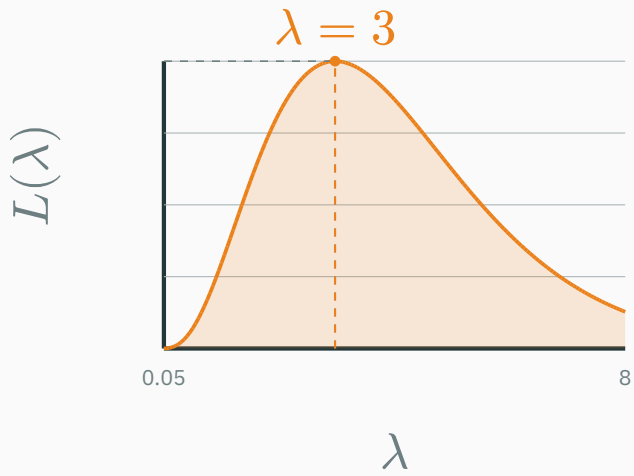

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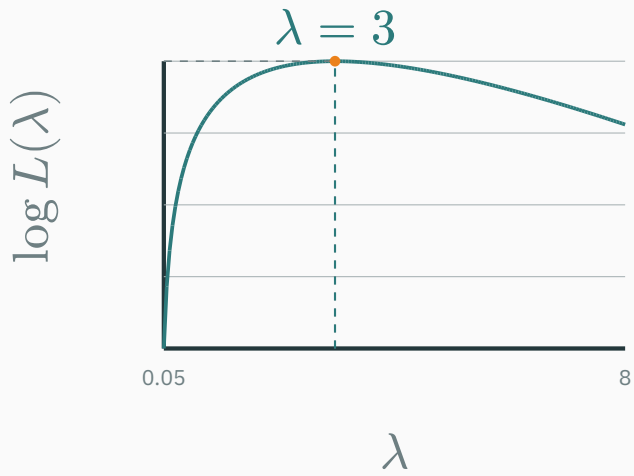

Both curves peak at $\hat{\lambda}_{\text{MLE}} = 3$: the log changes the vertical scale, not the maximizing parameter.

Why logs? Products become stable sums

D DERIVATION

For independent observations,

$$L(\boldsymbol{\theta}) = \prod_i p_{\boldsymbol{\theta}}(y_i \mid \boldsymbol{x}_i) \quad \Longrightarrow \quad \log L(\boldsymbol{\theta}) = \sum_i \log p_{\boldsymbol{\theta}}(y_i \mid \boldsymbol{x}_i)$$

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Worked numerical example. Suppose 200 observed outcomes each receive probability 0.01.

Direct product	$L = 0.01^{200} = 10^{-400} < 4.94 \times 10^{-324}$ → underflows to 0
Log space	$\log L = 200 \log(0.01) \approx -921.03$ → finite and representable

Float64 range: $\pm 1.80 \times 10^{308}$ · smallest positive normal 2.23×10^{-308} · smallest subnormal 4.94×10^{-324}.

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Logs make optimization easier and prevent numerical underflow.

Coin flips: solve for the stationary point

D DERIVATION

For $L(\theta) = \theta^{n_H}(1-\theta)^{n_T}$, the log-likelihood is

$$\log L(\theta) = n_H \log \theta + n_T \log(1-\theta)$$

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Set the derivative to zero:

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$$\implies \theta^\star = \frac{n_H}{n_H + n_T} = \frac{4}{10} = 0.4$$

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$\theta^\star = 0.4$ **is a candidate optimum. Next, check the curvature.**

The second derivative confirms a maximum

D DERIVATION

Differentiate the log-likelihood again:

$$\frac{\mathrm{d}^2}{\mathrm{d}\theta^2} \log L(\theta) = -\frac{n_H}{\theta^2} - \frac{n_T}{(1-\theta)^2}$$

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For $n_H, n_T > 0$ and $0 < \theta < 1$, both terms are negative:

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At the stationary point $\theta^\star = 0.4$,

$$-\frac{4}{(\quad)^2} - \frac{6}{(\quad)^2} = -25 - 16.67 \approx -41.67 < 0$$

The second derivative is negative everywhere, so the curve bends downward (is strictly concave). Its one stationary point is the unique global maximum: $\hat{\theta}_{\mathrm{MLE}} = 0.4$.

Maximizing likelihood = minimizing NLL

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Empirical risk = average training loss

D DERIVATION

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Per example	$\ell_{i(\boldsymbol{\theta})} = -\log p_{\boldsymbol{\theta}}(y_i \mid \boldsymbol{x}_i)$
Training set	$\hat{R}(\boldsymbol{\theta}) = \frac{1}{n}\sum_i \ell_{i(\boldsymbol{\theta})} = -\frac{1}{n}\log p(\mathcal{D} \mid \boldsymbol{\theta})$

The final equality uses conditional independence: $p(\mathcal{D}|\boldsymbol{\theta}) = \prod_i p_{\boldsymbol{\theta}}(y_i|\boldsymbol{x}_i)$.

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Minimizing empirical NLL is maximum likelihood; $\frac{1}{n}$ only rescales the objective.

Worked example: support becomes a hard loss

D DERIVATION

Recall the Uniform observation model:

$$p_{\boldsymbol{\theta}}(y_i \mid \boldsymbol{x}_i) = \begin{cases} 1/(b-a) & a \le y_i \le b \\ 0 & \text{otherwise} \end{cases}$$

Worked example: support becomes a hard loss

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Zero likelihood becomes an infinite training penalty.

Checkpoint: uniform support

Q QUESTION

For a Uniform(a, b) observation model, what is the NLL if the target lies outside $[a, b]$?

A. 0

B. A fixed finite penalty

C. $-\log 0 = +\infty$

D. It depends only on σ

Answer: uniform support

A ANSWER

Correct: C — $-\log 0 = +\infty$

Why: The model assigns zero density outside its support, so the observation is impossible under the assumption.

Regression: why MSE?

Regression as signal plus noise

$$y_i = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i) + \varepsilon_i, \qquad \varepsilon_i \sim \mathcal{N}(0, \sigma^2)$$

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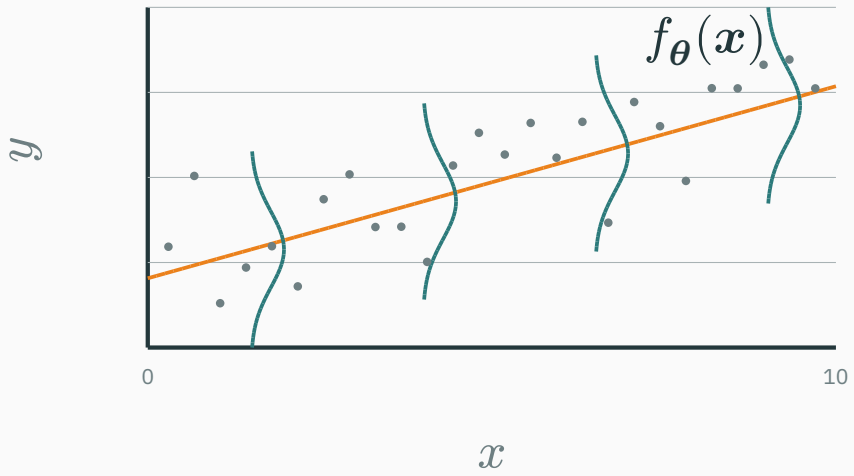
$$y_i = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i) + \varepsilon_i, \qquad \varepsilon_i \sim \mathcal{N}(0, \sigma^2)$$

Therefore the conditional output distribution is

$$Y_i \mid \boldsymbol{X}_i = \boldsymbol{x}_i \sim \mathcal{N}(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \sigma^2)$$

What the assumption means visually

V VISUAL



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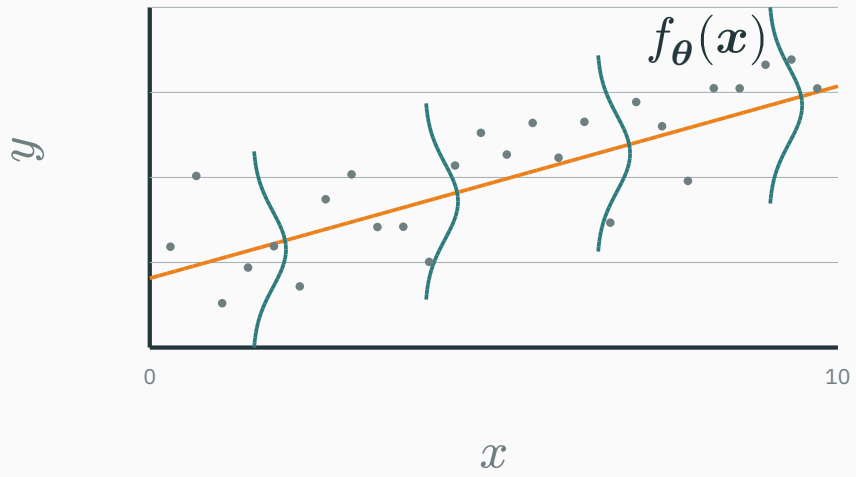

Gaussian noise lives in the **output direction**, conditional on x — a vertical bell at every input.

Gaussian likelihood

D DERIVATION

$$p_{\boldsymbol{\theta}}(y_i \mid \boldsymbol{x}_i) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{\left(y_i - f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)\right)^2}{2\sigma^2} \right)$$

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Negative log of a single example:

$$-\log p_{\boldsymbol{\theta}}(y_i \mid \boldsymbol{x}_i) = \frac{\left(y_i - f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)\right)^2}{2\sigma^2} + C$$

MSE is Gaussian MLE

Sum over the dataset:

$$-\log p(\mathcal{D} \mid \boldsymbol{\theta}) = \frac{1}{2\sigma^2} \sum_i \left(y_i - f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)\right)^2 + C$$

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With σ fixed, the minimizer is

$$\hat{\boldsymbol{\theta}}_{\mathrm{MLE}} = \arg\min_{\boldsymbol{\theta}} \sum_i \left(y_i - f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)\right)^2$$

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MSE = Gaussian NLL, up to constants.

Linear regression makes f_θ explicit

D DERIVATION

For the one-dimensional picture,

$$\hat{y}_i = \theta_0 + \theta_1 x_i$$

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For d features, prepend a constant 1 so the intercept is part of the same parameter vector:

$$\tilde{\boldsymbol{x}}_i = (1, \boldsymbol{x}_i), \quad \boldsymbol{\theta} = (\theta_0, \theta_1, \ldots, \theta_d)$$

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Then the same notation used throughout the lecture becomes

$$\hat{y}_i = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i) = \boldsymbol{\theta}^\top \tilde{\boldsymbol{x}}_i$$

θ_0 is the intercept; $\theta_1, \ldots, \theta_d$ are the slopes.

Gaussian MLE becomes ordinary least squares

D DERIVATION

Substitute the linear mean into the observation model:

$$Y_i \mid \boldsymbol{X}_i = \boldsymbol{x}_i \sim \mathcal{N}(\boldsymbol{\theta}^\top \tilde{\boldsymbol{x}}_i, \sigma^2)$$

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The vertical residual of point i is

$$r_i = y_i - \hat{y}_i = y_i - \boldsymbol{\theta}^\top \tilde{\boldsymbol{x}}_i$$

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With σ fixed, maximum likelihood therefore gives

$$\hat{\boldsymbol{\theta}}_{\mathrm{MLE}} = \arg\min_{\boldsymbol{\theta}} \sum_i \underbrace{r_i^2}_{\text{squared vertical error}}$$

Ordinary least squares is Gaussian maximum likelihood for a linear mean.

The normal equations solve linear regression

D DERIVATION

Stack the augmented inputs into $\tilde{\boldsymbol{X}} = [\mathbf{1} \quad \boldsymbol{X}]$. Then

$$\hat{\boldsymbol{y}} = \tilde{\boldsymbol{X}}\boldsymbol{\theta}, \quad J(\boldsymbol{\theta}) = \left\|\boldsymbol{y} - \tilde{\boldsymbol{X}}\boldsymbol{\theta}\right\|_2^2$$

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$$\nabla_{\boldsymbol{\theta}} J = 2\tilde{\boldsymbol{X}}^\top\left(\tilde{\boldsymbol{X}}\boldsymbol{\theta} - \boldsymbol{y}\right) = \mathbf{0}$$

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If $\tilde{\boldsymbol{X}}^\top \tilde{\boldsymbol{X}}$ is invertible,

$$\hat{\boldsymbol{\theta}} = \left(\tilde{\boldsymbol{X}}^\top \tilde{\boldsymbol{X}}\right)^{-1} \tilde{\boldsymbol{X}}^\top \boldsymbol{y}$$

Linear regression has a closed form; neural networks keep the MSE objective but use iterative optimization.

Why earlier ML courses could ignore σ^2

Q QUESTION

σ^2 is the observation-noise variance: the expected squared spread of targets around the mean prediction.

For n Gaussian observations, write $r_i = y_i - \mu_i$. The dataset NLL is

$$\mathcal{L}(\boldsymbol{\theta}; \sigma^2) = \frac{1}{2\sigma^2} \sum_i r_i^2 + \frac{n}{2} \log \sigma^2 + C.$$

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For point predictions, fixed-variance Gaussian MLE gives the same fitted model as MSE.

How is σ^2 chosen in practice?

D DERIVATION

One global noise level.

Fit the mean model, then estimate the residual spread:

$$\hat{\sigma}^2_{\text{MLE}} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{\mu}_i)^2.$$

Use this when a residual plot has roughly the same vertical width across inputs.

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Input-dependent noise.

Let the network predict both

$$(\mu_i, s_i) = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i),$$

$$s_i = \log \sigma_i^2, \quad \sigma_i^2 = e^{s_i} > 0.$$

Use this when residual spread changes with the input—for example, a funnel shape.

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Fit both cases with Gaussian NLL; validate interval coverage: the fraction of targets contained by intervals claiming a stated probability.

Homoscedastic vs input-dependent uncertainty

V VISUAL

HOMOSCEDASTIC

Network output: μ_i

Shared variance: σ^2

same uncertainty at every x_i

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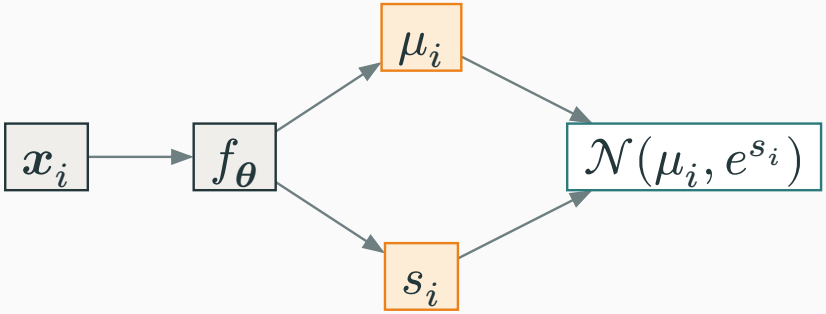

Network outputs: μ_i and s_i

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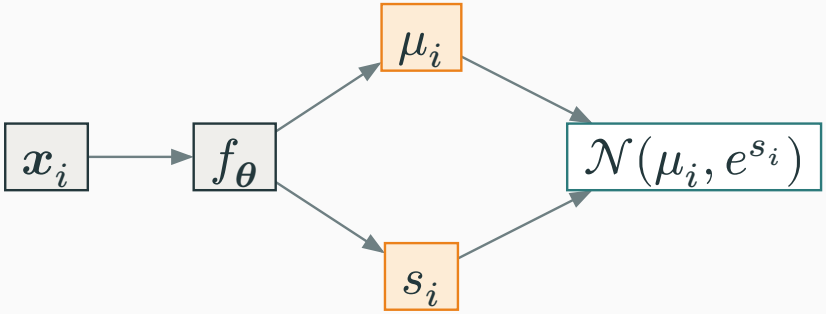


Network outputs: μ_i and s_i

$$s_i = \log \sigma_i^2, \quad \sigma_i^2 = e^{s_i} > 0$$

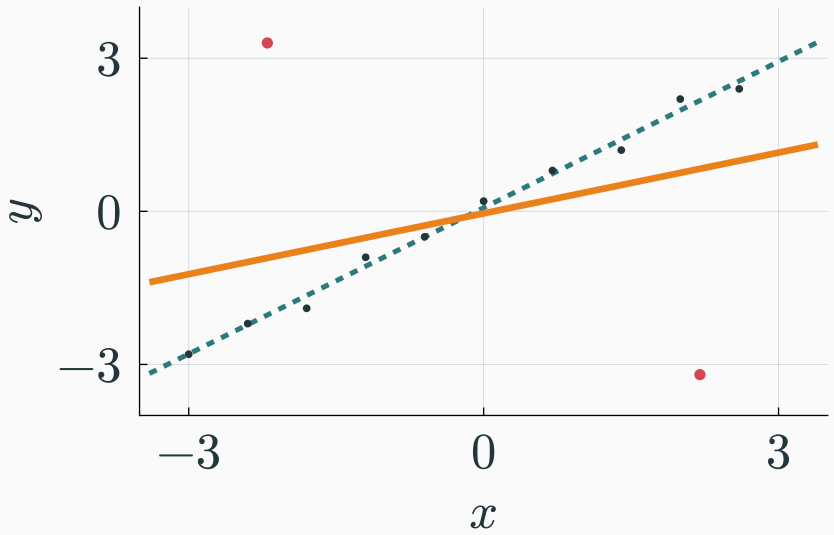
uncertainty changes with x_i

Predict log-variance so every real s_i maps to a positive variance e^{s_i}.

A few unusual observations can dominate a fitted line

Q QUESTION

SYNTHETIC · COMPUTED · exact 12-point teaching case; reproduced in the executed robust-notebook appendix



fit to the ten typical points MSE fit after adding two outliers

Ten typical observations lie near one linear trend.

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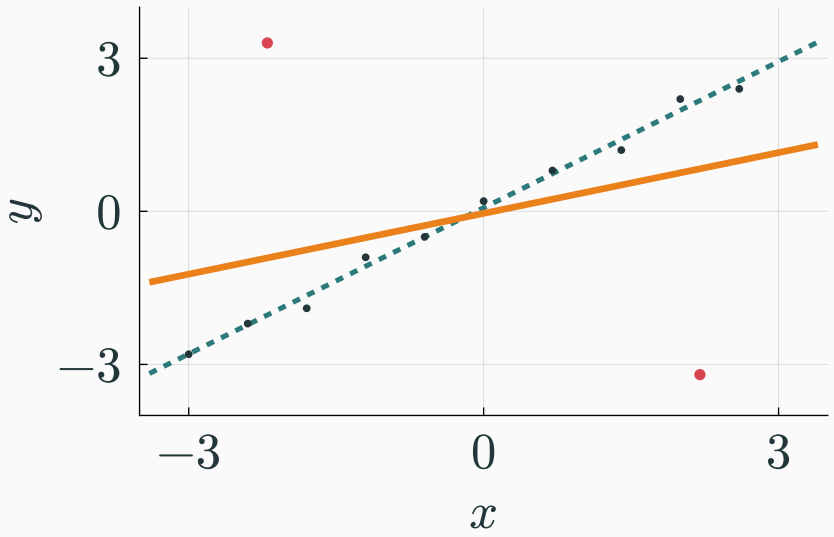

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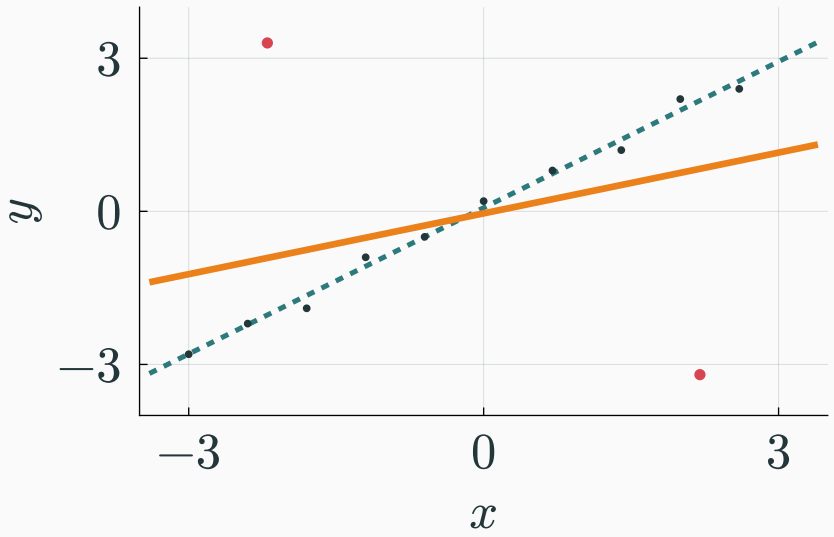


fit to the ten typical points MSE fit after adding two outliers

Ten typical observations lie near one linear trend.

Two unusual observations have large vertical errors.

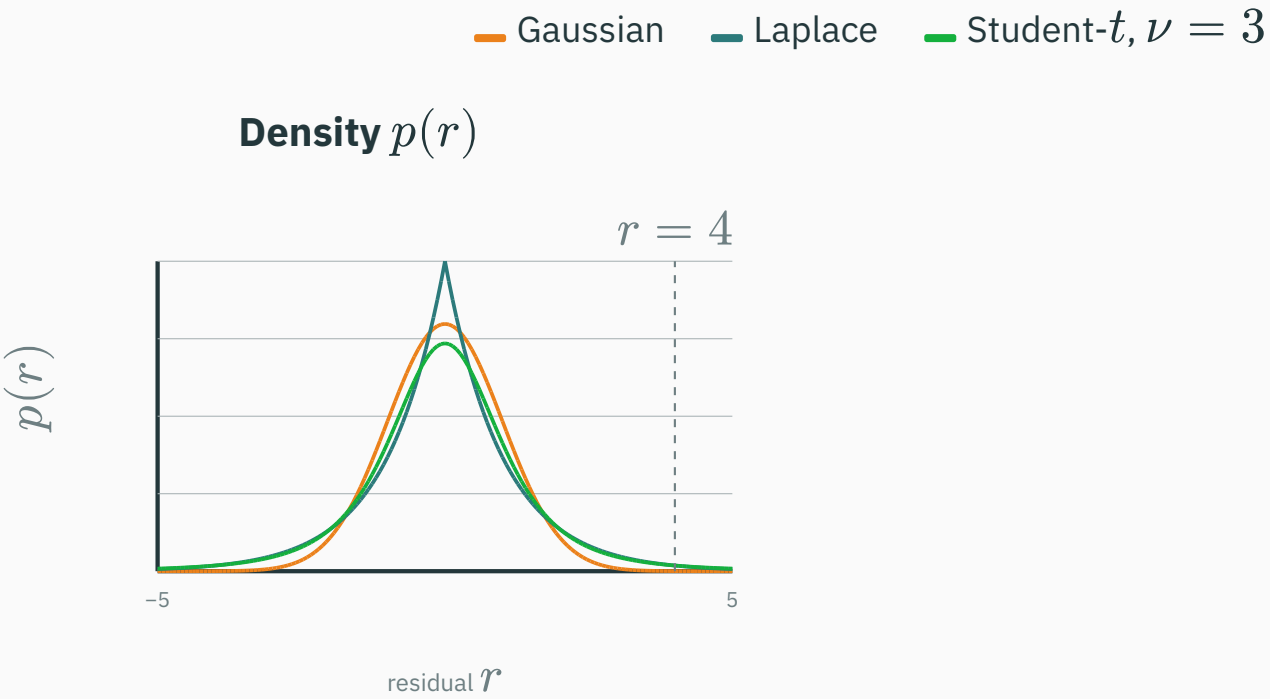
The squared-error fit becomes much flatter. How can two points change the fitted line so strongly?

Robust regression asks for a noise model that allows occasional large residuals without letting them dominate the fit.

Tails are easier to compare on a log scale

V VISUAL

For residual $r = y - \hat{y}$, compare unit-scale Gaussian, Laplace, and Student-t; $\nu = 3$ is its degrees of freedom.



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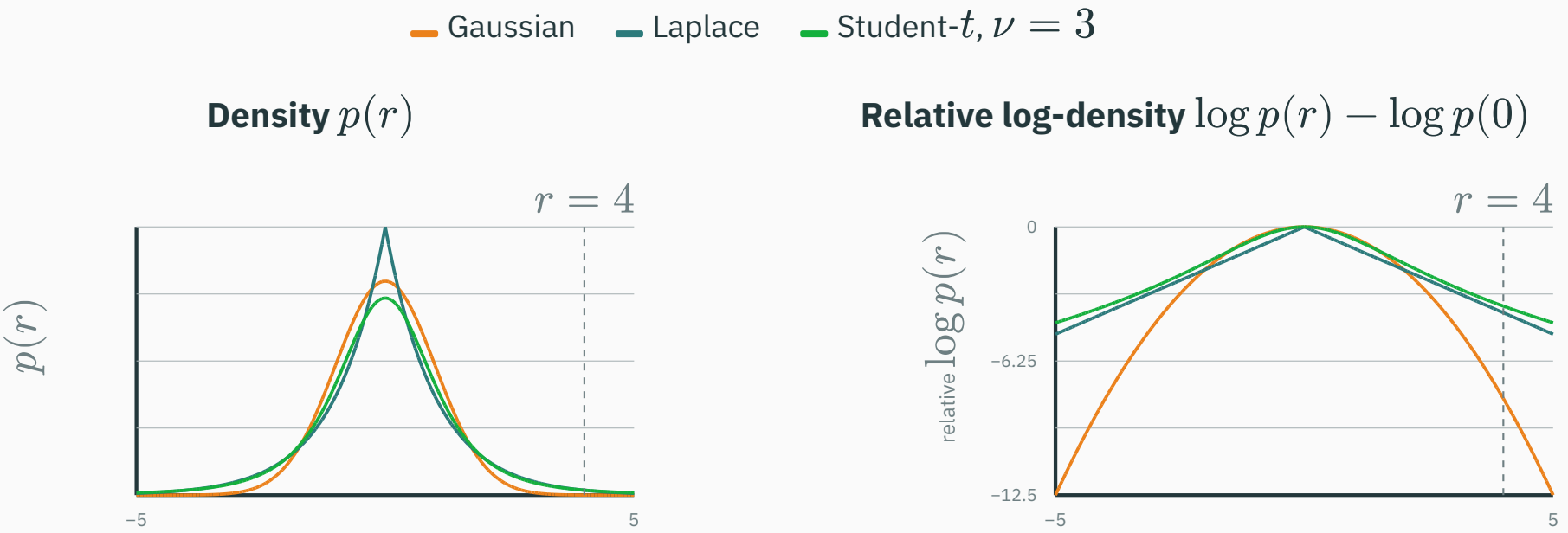

Smaller ν means heavier Student-t tails. Heavy tails make an occasional large residual less surprising.

A large residual is less surprising under heavy tails

D DERIVATION

Evaluate the three densities at the same residual, $r = 4$, using unit scale parameters.

Gaussian

density ≈ 0.000134

The model finds this residual extremely surprising.

Laplace

density ≈ 0.00916

More tail density makes the same residual less surprising.

Student-t, $\nu = 3$

density ≈ 0.00916

Heavy tails explicitly allow occasional extreme errors.

Laplace and Student-t assign about $68\times$ the Gaussian density here.

The observation is not discarded; the assumed noise process simply says that such an error can occur.

One observation contributes one gradient signal

D DERIVATION

For observation i, the model predicts $\hat{y}_i$ and leaves residual $r_i = y_i - \hat{y}_i$.

Loss value ℓ_i

says how incompatible this observation
is with the current prediction.

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Gradient magnitude $|\ell_{i'}(r_i)|$

says how strongly this observation scales the next parameter update.

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says how strongly this observation scales the next parameter update.

$$\nabla_{\boldsymbol{\theta}} \ell_i = -\ell_{i'}(r_i) \nabla_{\boldsymbol{\theta}} \hat{y}_i$$

The sign gives the correction direction; $|\ell_{i'}(r_i)|$ gives the size of this observation's gradient factor.

Residual density → NLL → parameter gradient

D DERIVATION

For one observation, $\hat{y}_i = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$ and $r_i = y_i - \hat{y}_i$.

$$\ell(r) = -\log p_{R(r)} \quad \rightarrow \quad \psi(r) = \mathrm{d}\frac{\ell}{\mathrm{d}r} = -\frac{1}{p_{R(r)}}\,\mathrm{d}\frac{p_{R(r)}}{\mathrm{d}r}$$

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$$\boxed{\nabla_{\boldsymbol{\theta}} \ell_i = \psi(r_i)\nabla_{\boldsymbol{\theta}} r_i = -\psi(r_i)\nabla_{\boldsymbol{\theta}} f_{\boldsymbol{\theta}}(\boldsymbol{x}_i).}$$

chain rule: residual-loss derivative × residual-to-model derivative

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chain rule: residual-loss derivative × residual-to-model derivative

Linear example: $f_{\boldsymbol{\theta}}(x) = \theta_0 + \theta_1 x \quad \rightarrow \quad \nabla_{\boldsymbol{\theta}} \ell_i = -\psi(r_i)(1, x_i)^\top.$

The density chooses $\psi(r)$; the model supplies $\nabla_\theta f$. Their product is the observation's parameter gradient.

Gaussian and Laplace residuals: the full chain

D DERIVATION

Noise	Residual density $p_{R(r)}$	NLL $\ell(r)$	$\psi(r) = \ell'(r)$
Gaussian	$\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{r^2}{2\sigma^2}}$	$\frac{r^2}{2\sigma^2} + C$	$\frac{r}{\sigma^2}$
Laplace	$\frac{1}{2s_L} e^{-\frac{\lvert r\rvert}{s_L}}$	$\frac{\lvert r\rvert}{s_L} + C$	$\frac{\operatorname{sign}(r)}{s_L}$

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Laplace	$\frac{1}{2s_L} e^{-\frac{\lvert r\rvert}{s_L}}$	$\frac{\lvert r\rvert}{s_L} + C$	$\frac{\operatorname{sign}(r)}{s_L}$

$$\nabla_{\boldsymbol{\theta}} \ell_i = -\psi(r_i) \nabla_{\boldsymbol{\theta}} f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

At $r = 0$, $|r|$ has no single derivative; optimization uses any slope in $\left[-\frac{1}{s_L}, \frac{1}{s_L}\right]$, called a **subgradient**. Away from zero, the gradient magnitude is $\frac{1}{s_L}$.

Gaussian influence grows with $|r|$; Laplace influence has constant magnitude.

Student-t residual: the full chain

D DERIVATION

For degrees of freedom ν and scale s:

ν controls tail heaviness; $s > 0$ sets residual scale; $c_{\nu,s} > 0$ normalizes the density to integrate to 1.

density	$p_{R(r)} = c_{\nu,s}\left(1 + \frac{r^2}{\nu s^2}\right)^{-\frac{\nu+1}{2}}$
NLL	$\ell(r) = \frac{\nu+1}{2}\log\left(1 + \frac{r^2}{\nu s^2}\right) + C$
r derivative	$\psi(r) = \mathrm{d}\frac{\ell}{\mathrm{d}r} = (\nu+1)\frac{r}{\nu s^2 + r^2}$
θ gradient	$\nabla_{\boldsymbol{\theta}}\ell_i = -(\nu+1)\frac{r_i}{\nu s^2 + r_i^2}\nabla_{\boldsymbol{\theta}} f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$

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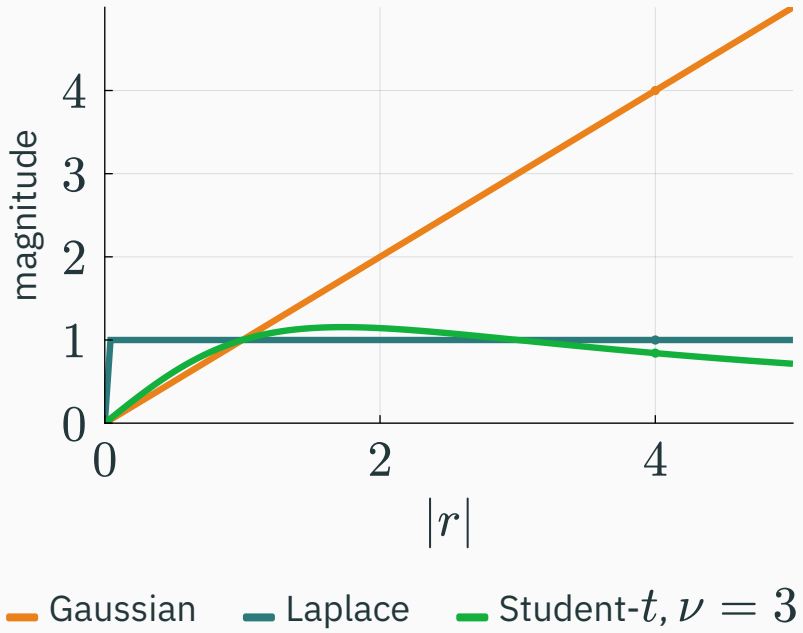
Near zero, $\psi(r) \approx \left(\frac{\nu+1}{\nu s^2}\right)r$; for $|r|$ very large, $\psi(r) \approx \frac{\nu+1}{r} \to 0$.

Student-t treats small residuals approximately quadratically, but an extreme residual's gradient contribution eventually decreases.

Large residuals create different gradient magnitudes

V VISUAL



At $r = 4$, the gradient factor is:

Gaussian

$|\ell'(4)| = 4$

Large residuals create different gradient magnitudes

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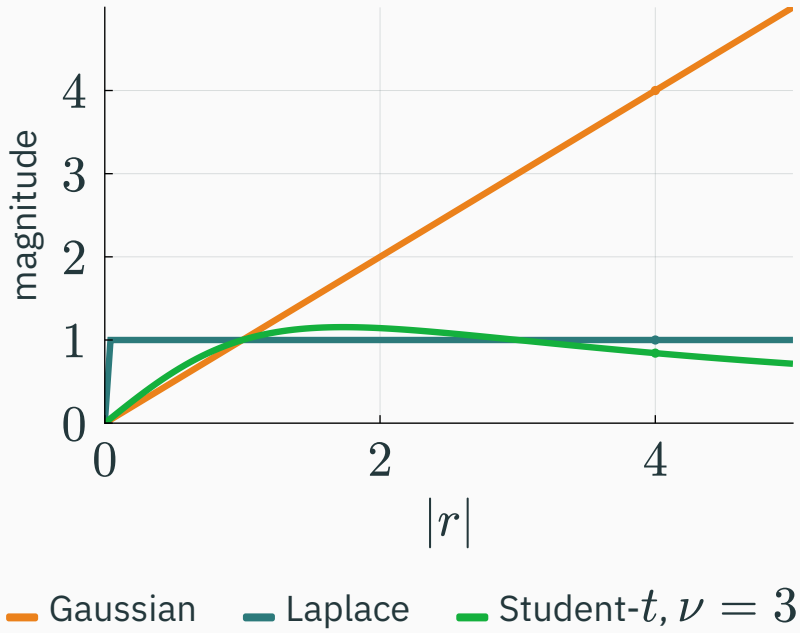

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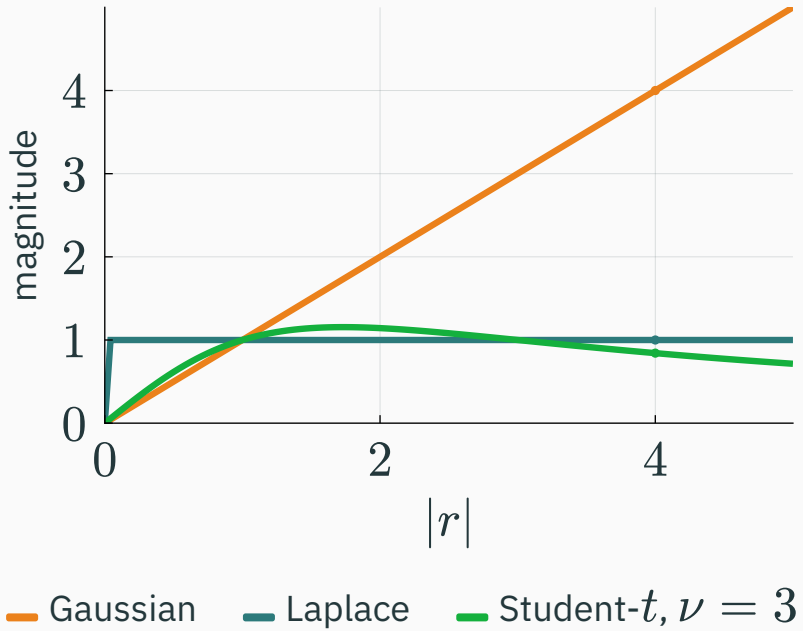

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Laplace

$$|\ell'(4)| = 1$$

Student-t

$$|\ell'(4)| = \tfrac{16}{19} \approx 0.84$$

Robust fitting keeps every observation, while limiting the gradient contribution of an extreme residual.

The noise model determines how errors are penalized

V VISUAL

Noise model	Negative log-likelihood
Gaussian	r^2
Laplace	$\lvert r \rvert$
Uniform	0 inside; $+\infty$ outside
Student-t	$\log\left(1 + \frac{r^2}{\nu}\right)$

$r = y - \hat{y}$ · swatches match plot

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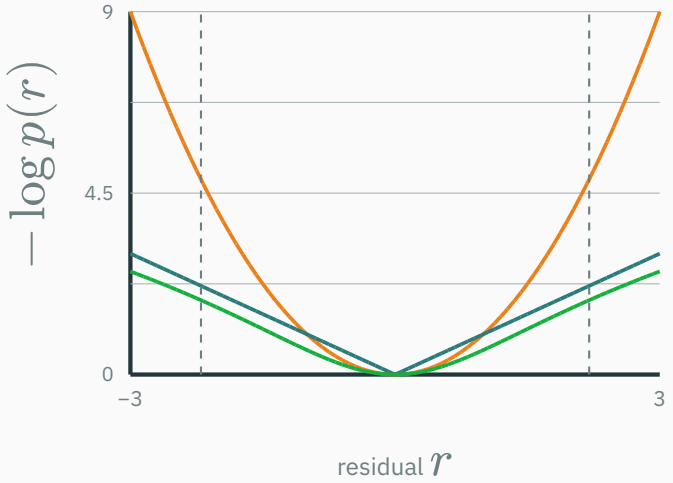

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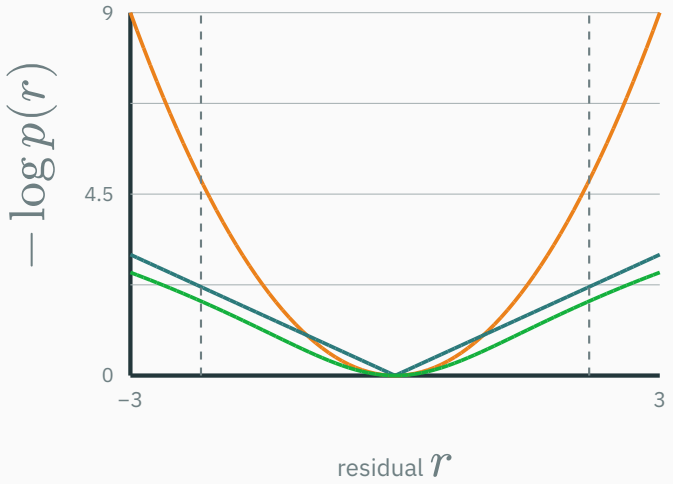

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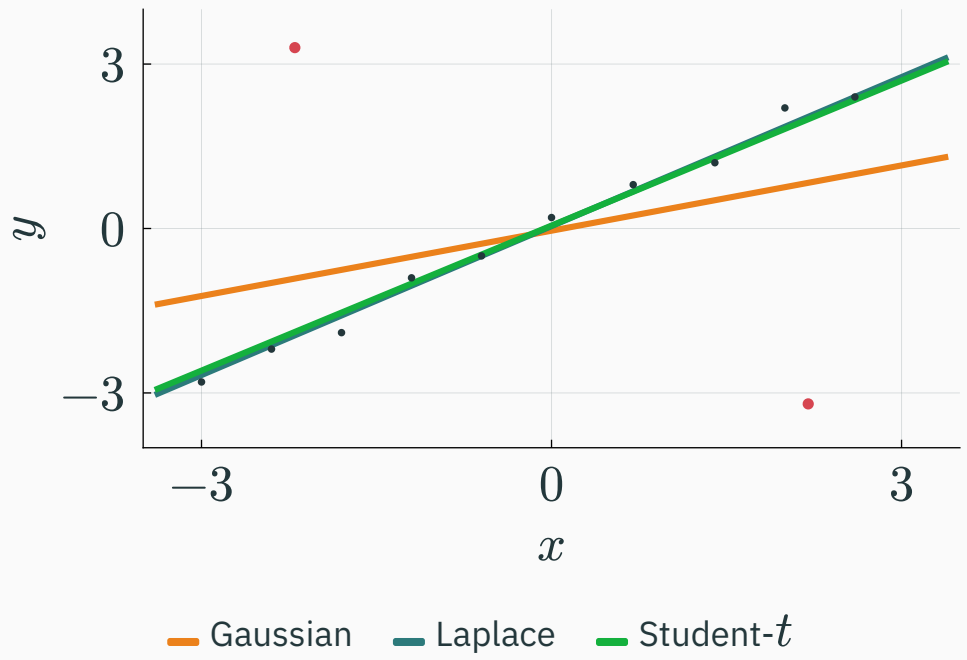
At $r = 0$, prediction equals target. Farther horizontally = larger error; higher vertically = larger NLL penalty.

Gaussian penalizes large errors most; Student-t is more robust. The dashed Uniform boundaries mark an infinite penalty outside the allowed interval.

Fit the same data under three noise models

V VISUAL



Learned $\hat{y} = \theta_0 + \theta_1 x$

model	fitted (θ_0, θ_1)
Gaussian	$(-0.040, 0.397)$
Laplace	$(0.044, 0.906)$
Student-t	$(0.053, 0.882)$

$$\sigma = 1 \cdot s_L = 1 \cdot (\nu, s) = (3, 1)$$

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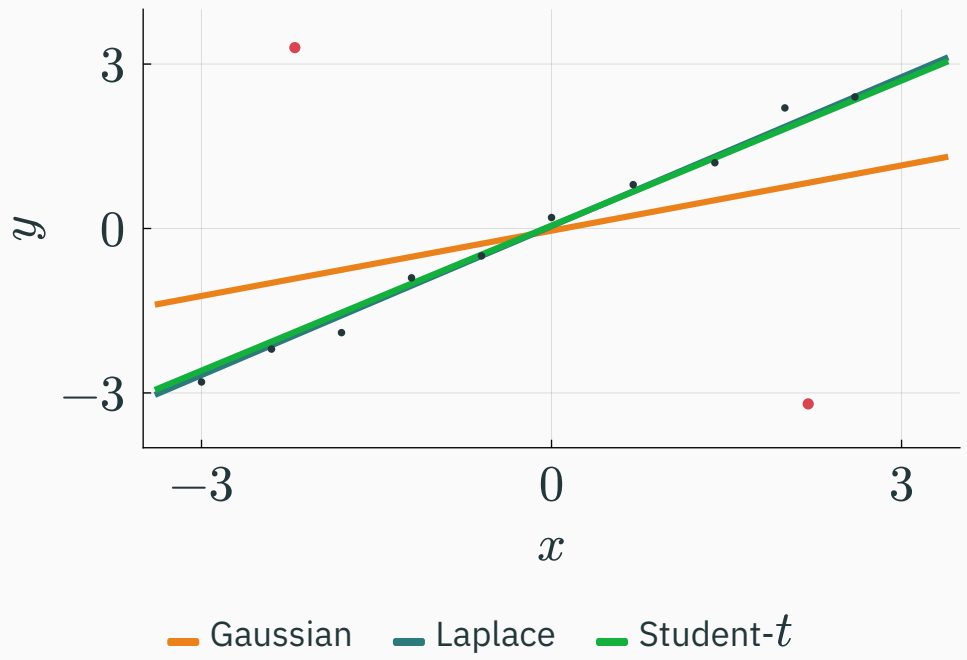

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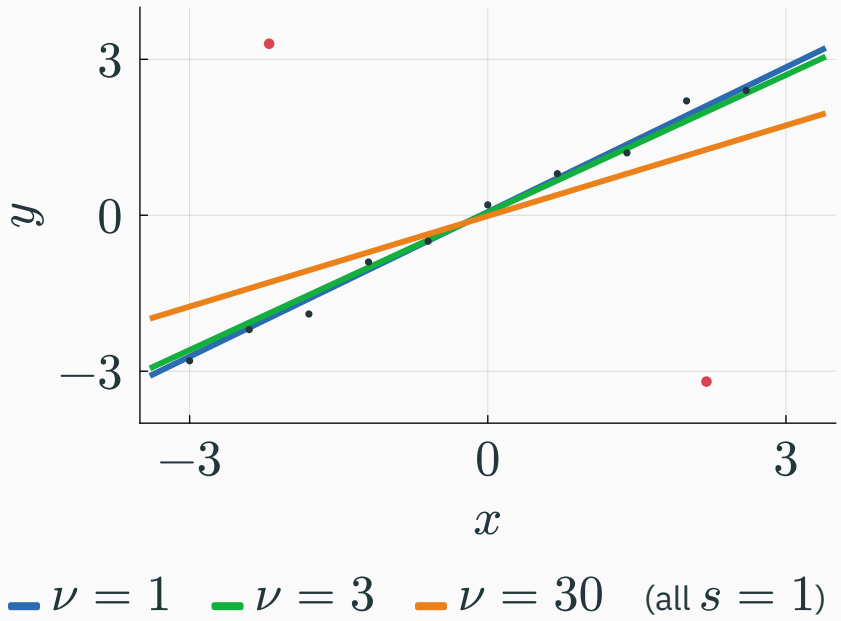
All twelve observations are retained. The models differ only in the residual likelihood optimized.

The Gaussian fit is pulled flat by the two red points; Laplace and Student-t stay close to the trend supported by the ten typical points.

Student-t hyperparameters control robustness

V VISUAL



Learned coefficients

ν	s	fitted (θ_0, θ_1)
1	1	$(0.064, 0.928)$
3	0.5	$(0.065, 0.934)$
3	1	$(0.053, 0.882)$
3	1.5	$(0.036, 0.807)$
30	1	$(-0.014, 0.581)$

Smaller ν gives heavier tails. Larger s delays the transition from quadratic to tail-robust behaviour.

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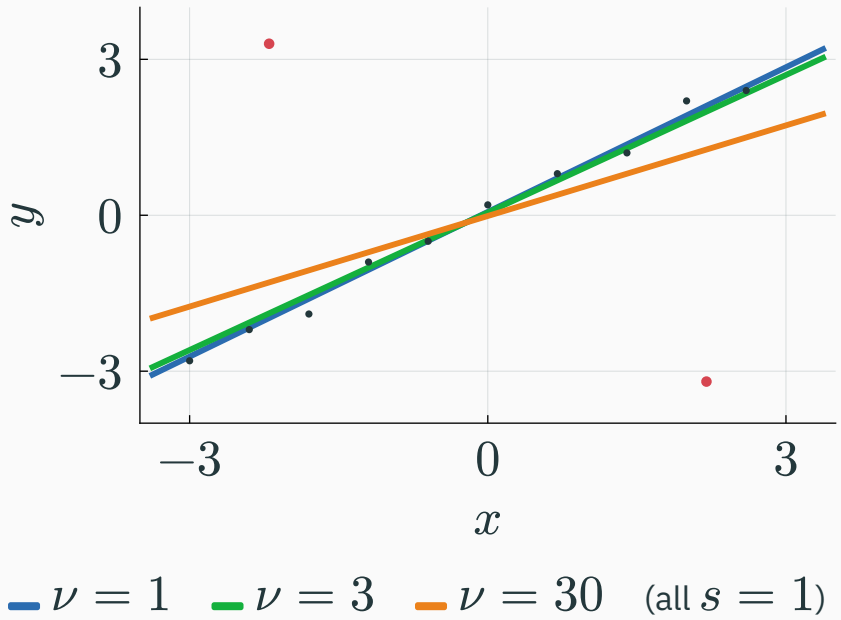

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Smaller ν gives heavier tails. Larger s delays the transition from quadratic to tail-robust behaviour.

For unregularized Gaussian and Laplace fits, changing the fixed scale only rescales the objective and leaves (θ_0, θ_1) unchanged; Student-t scale changes relative residual weights.

ν and s are modelling choices: cross-validation or domain knowledge should choose how quickly an observation is treated as a tail event.

Interactive: likelihood → loss

I INTERACTIVE

INTERACTIVE

↗ nipunbatra.github.io/interactive-articles/likelihood-to-loss

likelihood-to-loss.html — three synchronized panels: the **noise density** $p(r)$, the **loss** $-\log p(r)$, and **data with a fitted line**.

Controls: Gaussian / Laplace / Uniform / Student-t · noise scale · slope & intercept · **add an outlier** · per-point contributions.

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Ask: which model reacts most to an outlier? why does Uniform give an infinite barrier? which loss is robust?

Classification: cross-entropy

Classification should output probabilities

For K classes:

$$p_{\boldsymbol{\theta}}(Y = k \mid \boldsymbol{x}) \geq 0, \qquad \sum_{k=1}^{K} p_{\boldsymbol{\theta}}(Y = k \mid \boldsymbol{x}) = 1$$

A network first produces unconstrained class scores, called **logits**; sigmoid or softmax converts them to probabilities. We derive both below.

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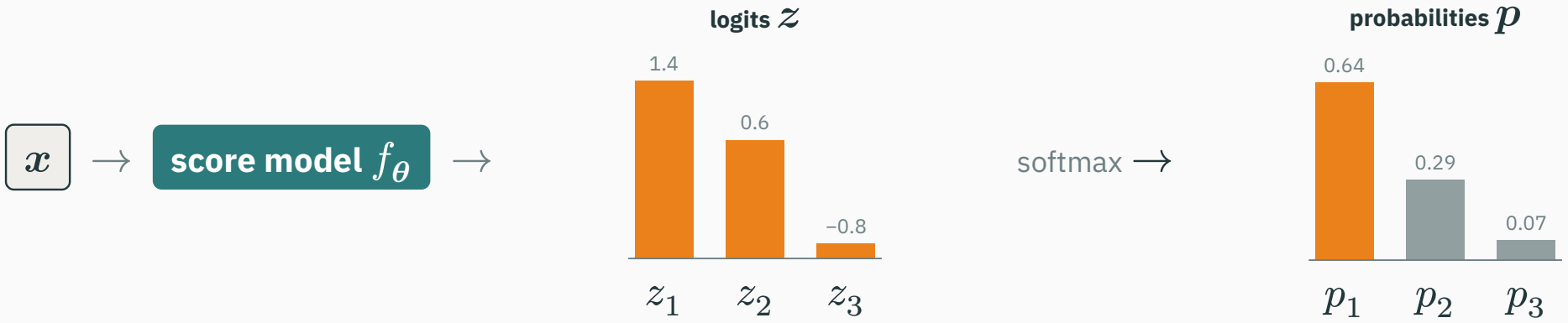

$f_{\boldsymbol{\theta}}$ may be linear or nonlinear; the probability constraints come from the output transformation.

Binary classification: Bernoulli model

$$Y \mid \boldsymbol{X} = \boldsymbol{x} \sim \text{Bernoulli}(p_{\boldsymbol{\theta}}(\boldsymbol{x}))$$

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$y = 1 \Rightarrow p(y) = p$

$y = 0 \Rightarrow p(y) = 1 - p$

Bernoulli NLL gives BCE

D DERIVATION

$$-\log p_{\boldsymbol{\theta}}(y \mid \boldsymbol{x}) = -\log\big(p^{y}(1-p)^{1-y}\big)$$

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Check. True label $y = 1$: if $p = 0.8$ the loss is $-\log 0.8 \approx 0.22$; if $p = 0.2$ it is $-\log 0.2 \approx 1.61$.

Why BCE matches a binary label better than MSE

For one observed example, let the target be $y = 1$ and the model predict

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Squared error

$$\ell_{\text{MSE}} = (y - p)^2 = (1 - 0.8)^2 = 0.04.$$

Its usual likelihood interpretation is Gaussian:

$$Y|\boldsymbol{x} \sim \mathcal{N}(0.8, \sigma^2).$$

Permits all real Y—not just labels.

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MSE is possible; BCE is the negative log-likelihood matched to a binary observation.

Why use logits?

V VISUAL

The network emits an unbounded score $z = f_{\boldsymbol{\theta}}(\boldsymbol{x}) \in \mathbb{R}$; the **sigmoid** maps it to a probability:

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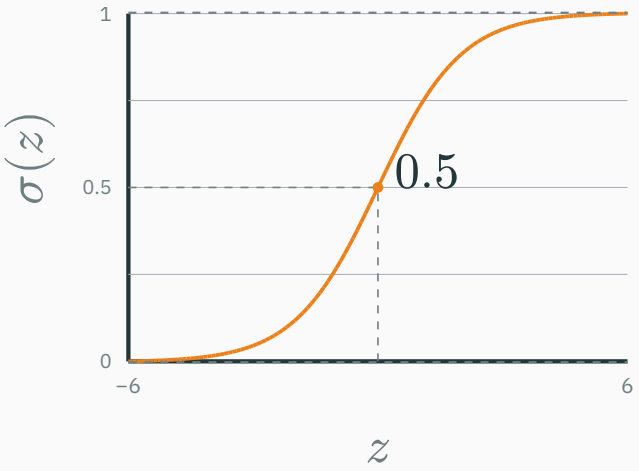
$z \to -\infty : p \to 0$
$z = 0 : p = 0.5$
$z \to +\infty : p \to 1$

In practice sigmoid + BCE are fused for numerical stability.



Logistic regression = Bernoulli MLE

D DERIVATION

Use an augmented input $\tilde{\boldsymbol{x}}_i$ so $\boldsymbol{\theta}$ contains both weights and the intercept:

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Logistic regression is Bernoulli maximum likelihood; its training objective is **binary cross-entropy**.

Multi-class model and softmax

V VISUAL

CATEGORICAL OBSERVATION

$$Y \mid \boldsymbol{X} = \boldsymbol{x} \sim \text{Categorical}(p_1, ..., p_K)$$

A **one-hot** target has one 1 at the true class and 0 everywhere else.

Example: class 2 of 3 $\rightarrow \boldsymbol{y} = (0, 1, 0)$

$$p_{\boldsymbol{\theta}}(\boldsymbol{y} \mid \boldsymbol{x}) = \prod_{k=1}^{K} p_k^{y_k}$$

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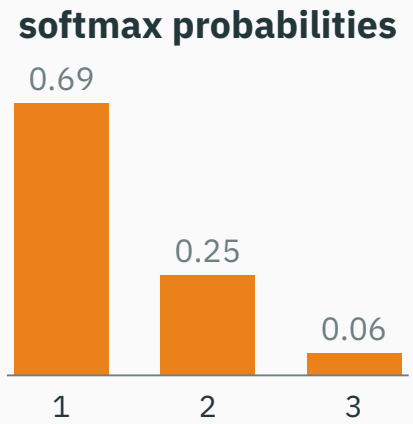

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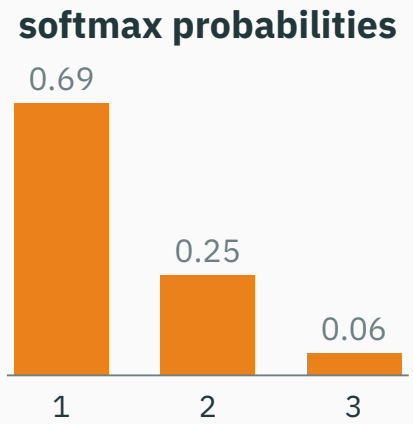

Softmax guarantees $p_k > 0$ and $\sum_k p_k = 1$, as a categorical model requires.

Categorical NLL gives cross-entropy

D DERIVATION

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Because $\boldsymbol{y}$ is one-hot, only the true class survives:

$$\mathcal{L} = -\log p_{\text{true class}}$$

Confident mistakes are expensive

V VISUAL

$$\ell(p_y) = -\log p_y$$

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Read off the loss at three confidences for the **true** class:

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Read off the loss at three confidences for the **true** class:

$$p_y = 0.9 \Rightarrow \ell \approx 0.105$$
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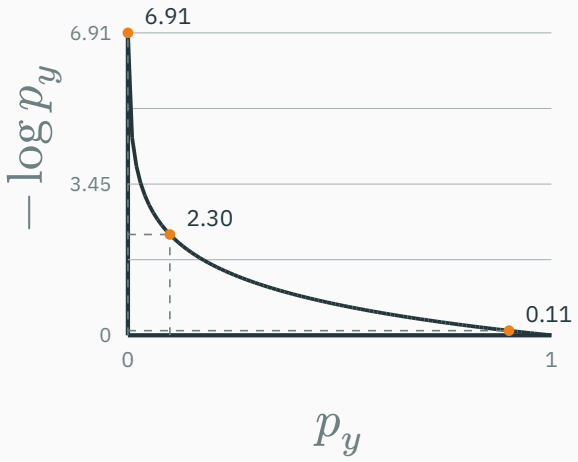

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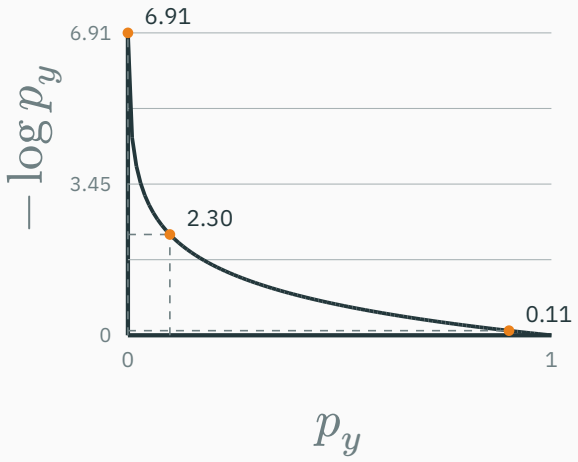

The negative log makes a confident wrong prediction a large loss.

Checkpoint: confident mistakes

Q QUESTION

Why does cross-entropy penalize a confidently wrong prediction strongly?

A. It makes all class probabilities equal

B. The true-class probability is near zero, so $-\log p_y$ is large

C. It adds an L_2 penalty to the logits

D. The gradient is always zero

Answer: confident mistakes

A ANSWER

Correct: B — The true-class probability is near zero

Why: The negative log grows without bound as p_y approaches zero, matching the fact that the model declared the observed class nearly impossible.

Bayes’ rule for learning

Bayes' rule: from events to model parameters

V VISUAL

PROBABILITY LECTURE

$$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B)}$$

A — event or hypothesis to infer

B — observed event or information

Examples: disease given a test; urn given a sampled colour.

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MACHINE / DEEP LEARNING

$$p(\boldsymbol{\theta} \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathcal{D})}$$

$p(\boldsymbol{\theta})$ — prior before seeing the dataset
$p(\mathcal{D}|\boldsymbol{\theta})$ — likelihood of the fixed dataset
$p(\mathcal{D})$ — evidence (normalizing constant)
$p(\boldsymbol{\theta}|\mathcal{D})$ — posterior after seeing the dataset

Question: which parameter settings remain plausible after seeing the data?

Bayes' rule: from events to model parameters

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$p(\boldsymbol{\theta})$ — prior before seeing the dataset
$p(\mathcal{D}|\boldsymbol{\theta})$ — likelihood of the fixed dataset
$p(\mathcal{D})$ — evidence (normalizing constant)
$p(\boldsymbol{\theta}|\mathcal{D})$ — posterior after seeing the dataset

Question: which parameter settings remain plausible after seeing the data?

Replace A by θ and B by $\mathcal{D}$: the algebra is unchanged; the interpretation changes.

Three heads do not prove $\theta = 1$

Q QUESTION

Let $\theta = P(H)$ and suppose the first three flips are $\mathcal{D} = (H, H, H)$.

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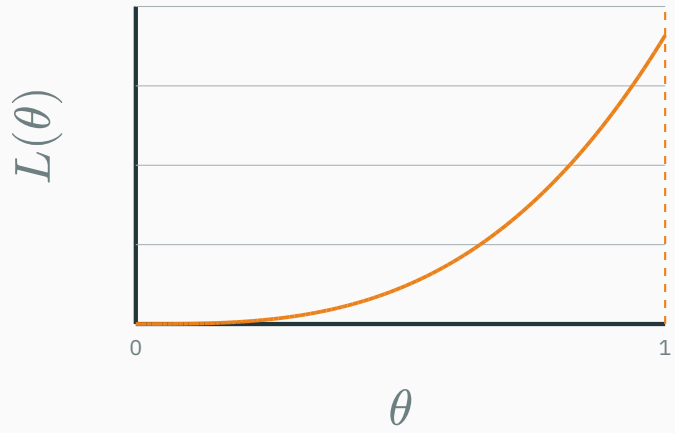
H · H · H

$$L(\theta; \mathcal{D}) = p(\mathcal{D} \mid \theta) = \theta^3$$

$$L(\theta) = \theta^3$$



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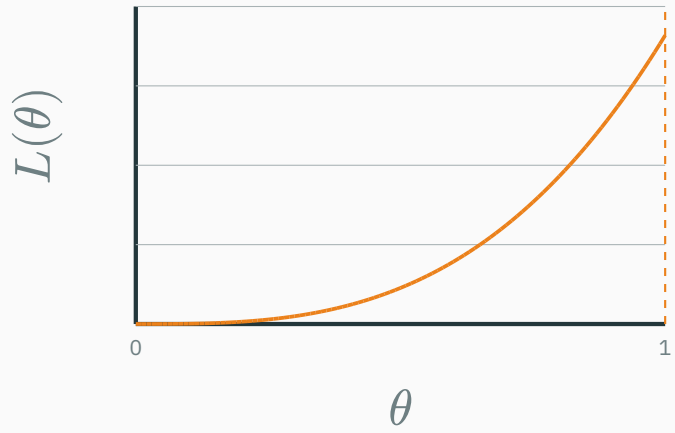

$$L(\theta; \mathcal{D}) = p(\mathcal{D} \mid \theta) = \theta^3$$

$$\hat{\theta}_{\text{MLE}} = \arg\max_{0 \le \theta \le 1} \theta^3 = 1$$

Did we learn that the coin **always** lands heads —or did a merely head-biased coin produce a lucky run?

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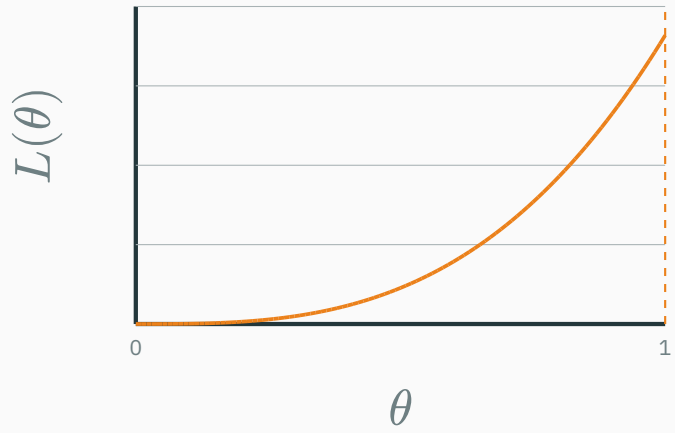

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MLE identifies the best-fitting θ; it does not make $\theta = 1$ certain.

A prior tempers the conclusion from three flips

V VISUAL

Choose a smooth prior on $\theta \in [0, 1]$, highest near the fair-coin value 0.5.

Prior

$$p(\theta) = 6\theta(1 - \theta)$$

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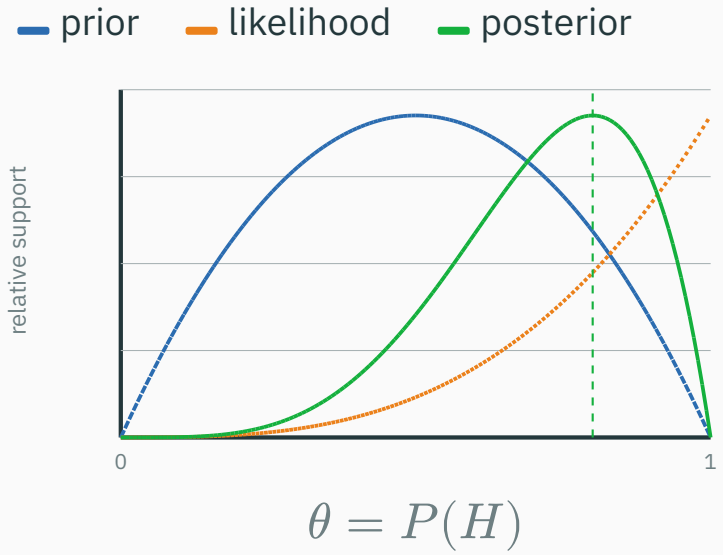
Posterior

$$p(\theta \mid \mathcal{D}) \propto \theta^3 p(\theta) \propto \theta^4(1 - \theta)$$

Likelihood peak (MLE): $\theta = 1$

Posterior peak: $\theta = \frac{4}{5} = 0.8$



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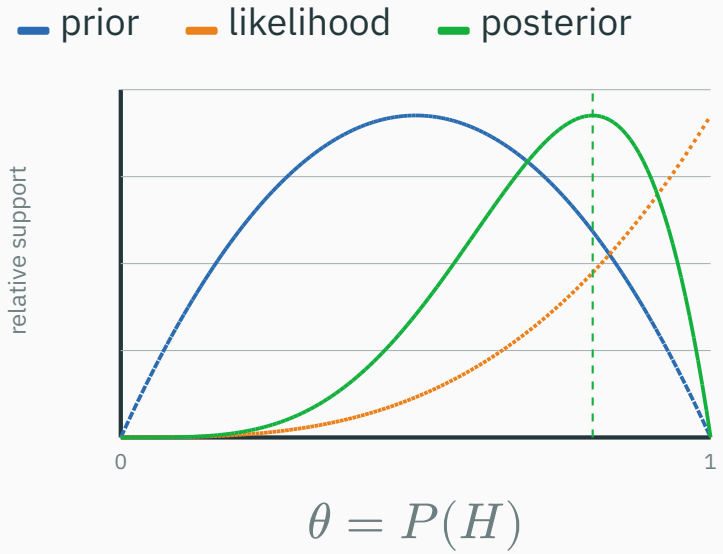

With little data, the prior matters; as observations accumulate, the likelihood increasingly dominates.

Step 1: fixed data give fixed likelihoods

D DERIVATION

Suppose we consider only two possible coins.

Fair coin F

$$P(H|F) = 0.5$$

Heads-biased coin B

$$P(H|B) = 0.9$$

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Observed data: H · H · H

$$P(H, H, H|F) = 0.5^3 = 0.125 \qquad P(H, H, H|B) = 0.9^3 = 0.729$$

$$\text{likelihood ratio} = \frac{0.729}{0.125} \approx 5.83$$

HHH favours B over F by a factor of 5.83. These likelihoods do not depend on the prior.

Step 2: update a prior that favours the fair coin

D DERIVATION

Before seeing the flips, suppose our starting belief is $P(F) = 0.90$ and $P(B) = 0.10$.

Hypothesis	Prior	Likelihood	Prior × likelihood
Fair F	0.90	0.125	$0.90 \times 0.125 = 0.1125$
Biased B	0.10	0.729	$0.10 \times 0.729 = 0.0729$

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$w_F = 0.1125$ and $w_B = 0.0729$ are **weights**, not probabilities yet.

Bayes first scores each hypothesis by prior $\times$ likelihood. The two scores need not add to 1.

Step 3: normalize the weights into probabilities

D DERIVATION

The normalizing constant is the sum of the two weights:

$$P(\mathcal{D}) = w_F + w_B = 0.1125 + 0.0729 = 0.1854.$$

$P(\mathcal{D})$ is the **evidence** (also called marginal likelihood); it makes posterior probabilities sum to 1.

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Fair coin

$$P(F|\mathcal{D}) = \frac{0.1125}{0.1854} \approx 0.607$$

Heads-biased coin

$$P(B|\mathcal{D}) = \frac{0.0729}{0.1854} \approx 0.393$$

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The normalized values now add to 1: $0.607 + 0.393 = 1$. They are the **posterior** probabilities—our beliefs after observing HHH.

HHH raises belief in B from 0.10 to 0.393, but it does not overturn the strong fair-coin prior.

Step 4: start instead from a biased-coin prior

D DERIVATION

Now use the **same hypotheses and the same HHH**, but start from $P(F) = 0.10$ and $P(B) = 0.90$.

Hypothesis	Prior	Likelihood	Weight
Fair F	0.10	0.125	0.0125
Biased B	0.90	0.729	0.6561

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Fair F	0.10	0.125	0.0125
Biased B	0.90	0.729	0.6561

$$P(\mathcal{D}) = 0.0125 + 0.6561 = 0.6686$$

$$P(F|\mathcal{D}) \approx 0.019, \quad P(B|\mathcal{D}) \approx 0.981$$

The data again favours B by the same factor 5.83; this time the prior already favoured B.

What changed—and what stayed fixed?

V VISUAL

Starting belief	**Prior** $P(B)$	**Posterior** $P(B\|H,H,H)$
Probably fair	0.10	0.393
Probably biased	0.90	0.981

What changed—and what stayed fixed?

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Fixed: the observations and likelihoods. In both analyses, HHH multiplies the odds for B by 5.83.

Changed: the prior. Different starting beliefs therefore lead to different posterior probabilities.

Odds for B versus F mean $\frac{P(B)}{P(F)}$.

posterior odds $=$ prior odds $\times$ likelihood ratio

Bayes does not erase the prior; it updates it with the same observations. More data makes the likelihood increasingly dominant.

Maximum a posteriori (MAP) estimation

D DERIVATION

$$\hat{\boldsymbol{\theta}}_{\mathrm{MAP}} = \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta} \mid \mathcal{D}) = \arg\max_{\boldsymbol{\theta}} p(\mathcal{D} \mid \boldsymbol{\theta})\, p(\boldsymbol{\theta})$$

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MAP objective: NLL + negative log-prior. In ML language: data loss + regularization.

Priors, MAP and regularization

Every learner has an inductive bias

V VISUAL

When several predictors fit the training data, the learner still needs a preference for **unseen inputs**. That preference is its **inductive bias**.

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Model	Built-in preference → consequence
Linear regression	responses vary linearly with features → line or plane extrapolation
k-NN	nearby inputs tend to have similar outputs → local prediction
Decision tree	a few axis-aligned rules partition the space → piecewise-constant regions
CNN	useful local patterns repeat across positions → shared filters recognize translations

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A prior is one explicit inductive bias; the model class, features, architecture, and optimization add others.

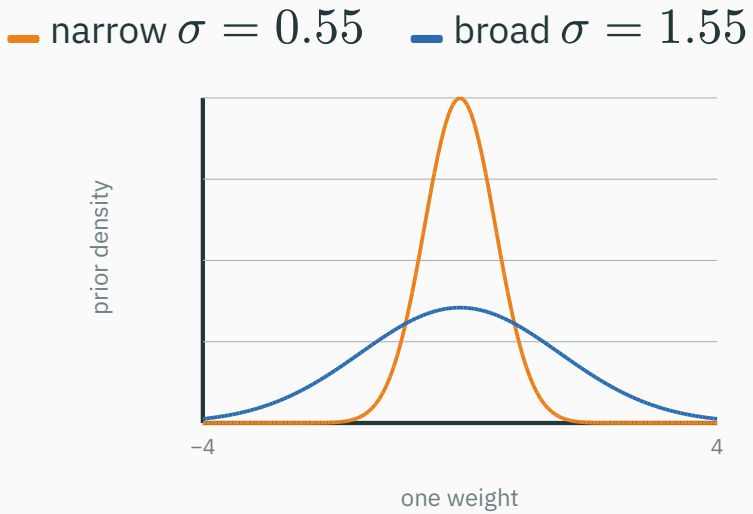
A neural-network prior ranks plausible parameter vectors

V VISUAL

$$\boldsymbol{\theta} \sim p(\boldsymbol{\theta})$$

For a neural network, $\boldsymbol{\theta}$ contains all weights and biases. Before using the current dataset, a prior states which settings are more plausible.

It can prefer small or sparse weights (**sparse** = many weights at or near zero), smooth functions, and correlated parameters.



narrow = stronger preference near 0

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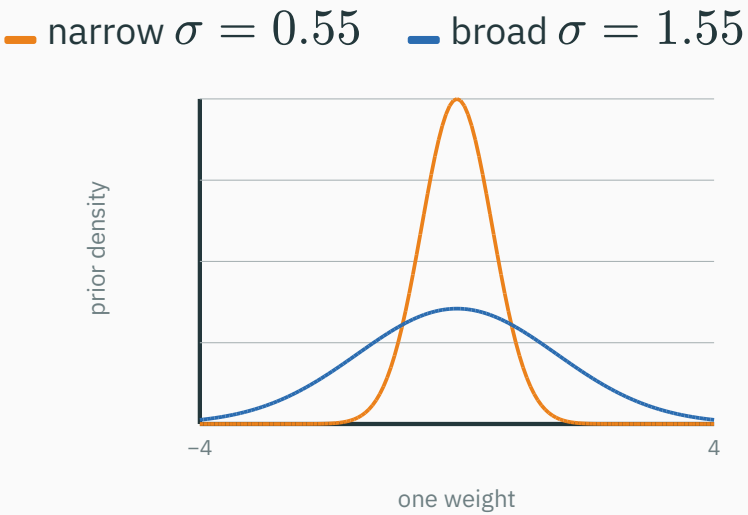

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A prior makes part of the model's inductive bias explicit as a probability distribution.

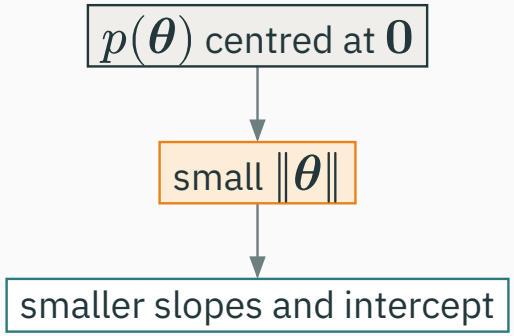
Parameter priors have visible consequences

V VISUAL

Example: a zero-centred prior makes parameter values near $\boldsymbol{\theta} = \mathbf{0}$ more plausible before seeing data.

REGRESSION

$$Y_i \mid \boldsymbol{X}_i = \boldsymbol{x}_i \sim \mathcal{N}(\boldsymbol{\theta}^\top \tilde{\boldsymbol{x}}_i, \sigma^2)$$



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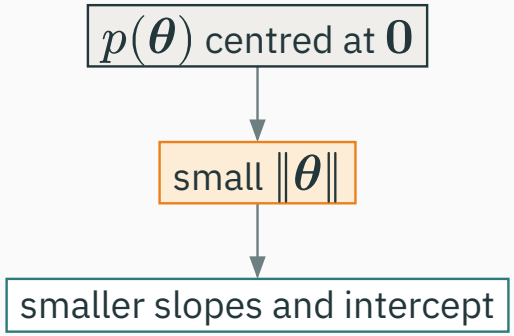
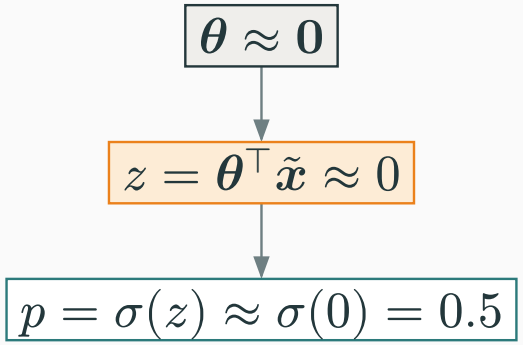


BINARY CLASSIFICATION

$$p_{\boldsymbol{\theta}}(Y = 1 \mid \boldsymbol{x}) = \sigma(\boldsymbol{\theta}^\top \tilde{\boldsymbol{x}})$$



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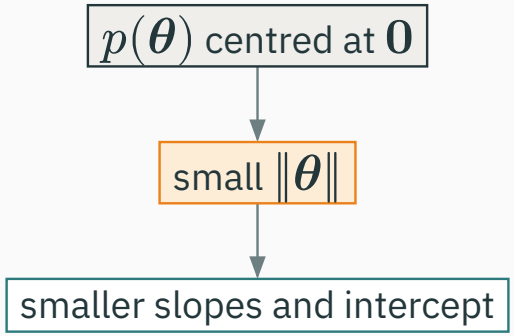

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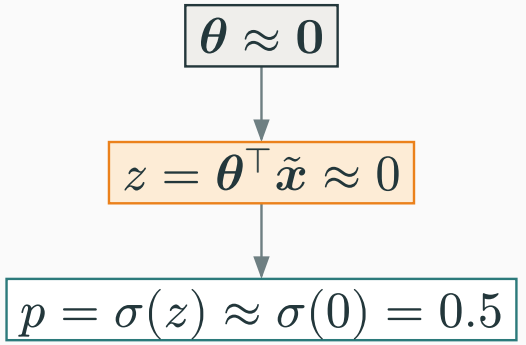


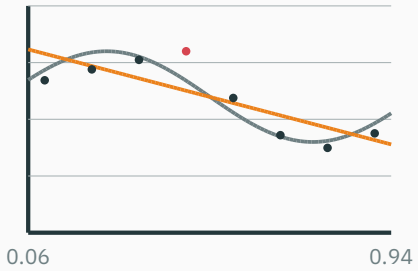
This conclusion depends on the prior: a prior centred elsewhere can prefer probabilities away from 0.5.

Model complexity: underfitting to overfitting

Fit the same eight observations by least squares; only the polynomial degree changes.

dashed = underlying trend · orange = fitted polynomial · red dot = one noisy observation

degree 1



x

underfit

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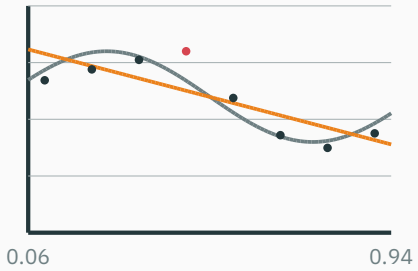
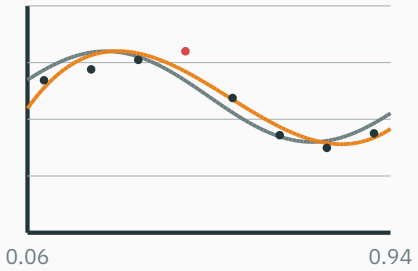


underfit

degree 3



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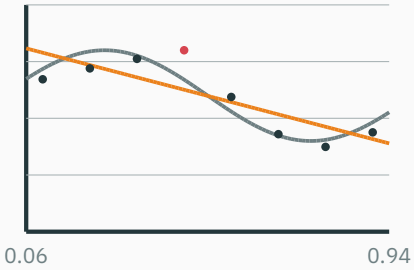

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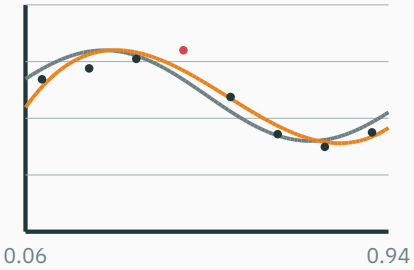

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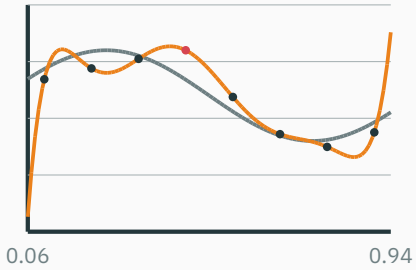
degree 7



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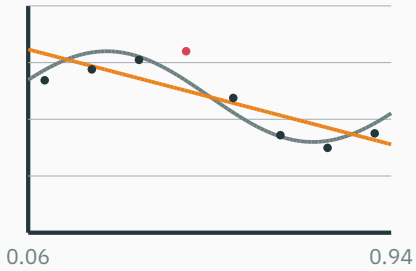

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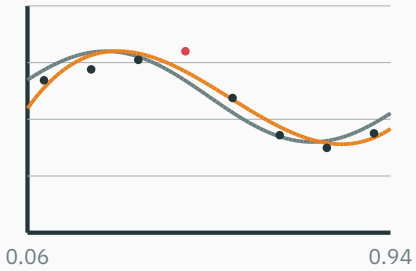

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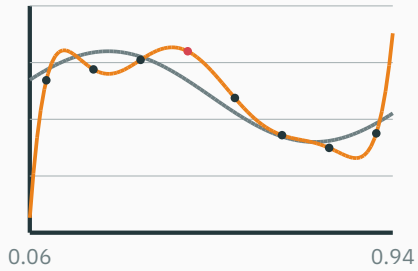

overfit

Higher degree lowers training error, but degree 7 chases the noisy observation and becomes unstable. Priors and regularization can prefer smoother solutions.

Start with four noisy points from a straight line

V VISUAL

The data were generated from $f_{\text{true}(x)} = 2 + 3x$ with small measurement noise.

x	$f_{\text{true}(x)}$	observed y
-1	-1	-0.8
0	2	1.8
1	5	5.3
2	8	7.9

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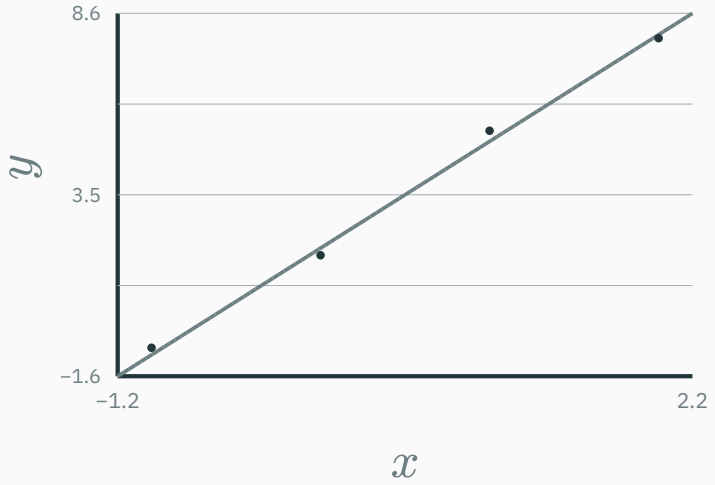

grey line = generating rule · dots = observed data

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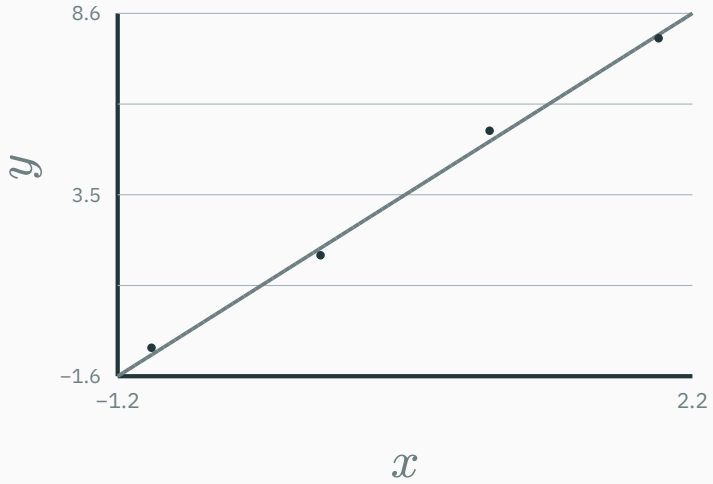

grey line = generating rule · dots = observed data

The learner sees only the four observations and must infer the intercept b and slope w.

The likelihood peaks near the generating line

D DERIVATION

Model each observation as

$$Y_i | x_i, b, w \sim \mathcal{N}(b + w x_i, 0.5^2).$$

The data score each candidate line

$$L(b, w) \propto \exp\left(-\frac{1}{2(0.5)^2} \sum_i (y_i - b - w x_i)^2 \right).$$

candidate (b, w)	squared error
$(2, 3)$	0.180
$(0, 1)$	56.580
MLE $(2.07, 2.96)$	0.162

The likelihood peaks near the generating line

D DERIVATION

Model each observation as

$$Y_i | x_i, b, w \sim \mathcal{N}(b + w x_i, 0.5^2).$$

The data score each candidate line

$$L(b, w) \propto \exp\left(-\frac{1}{2(0.5)^2} \sum_i (y_i - b - w x_i)^2 \right).$$

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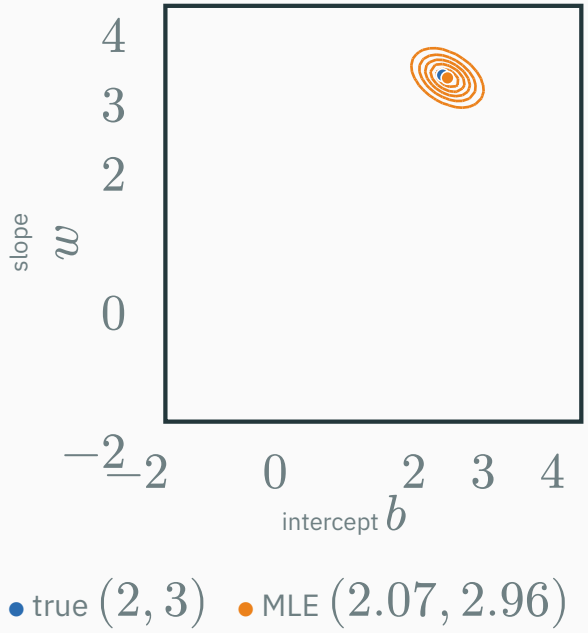

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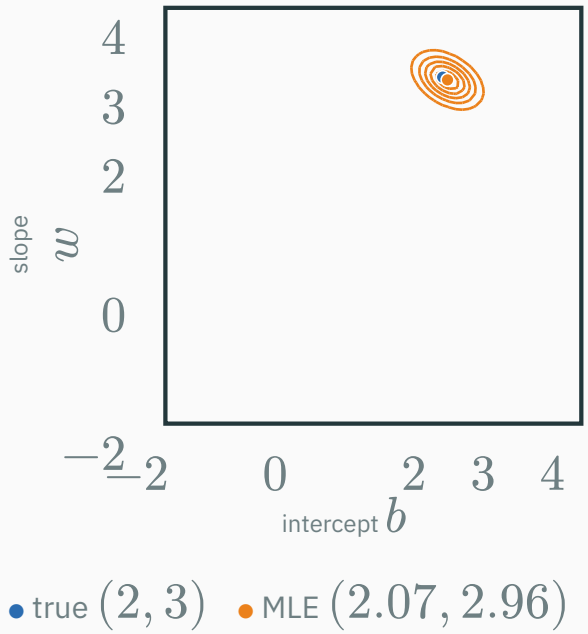

The observed data make intercepts near 2 and slopes near 3 most plausible.

Before data, the prior prefers parameters near zero

V VISUAL

Choose a simple Gaussian prior over the two regression parameters:

$$\boldsymbol{\theta} = (b, w) \sim \mathcal{N}(\mathbf{0}, \tau^2 \boldsymbol{I}), \quad \text{here } \tau = 0.5.$$

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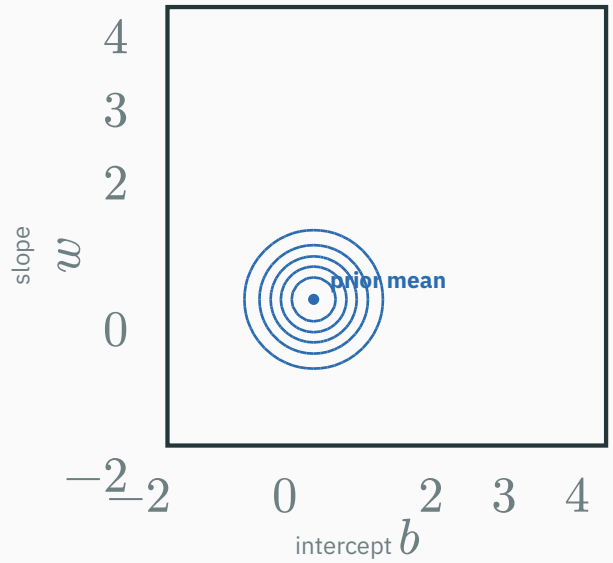

What does it express?

$$-\log p(b, w) = \tfrac{1}{2\tau^2}(b^2 + w^2) + C = 2(b^2 + w^2) + C \quad \text{when } \tau = 0.5.$$

Before seeing this dataset:

- $b \approx 0$ and $w \approx 0$: small-intercept, flatter lines
- farther from $(0, 0)$: less prior density

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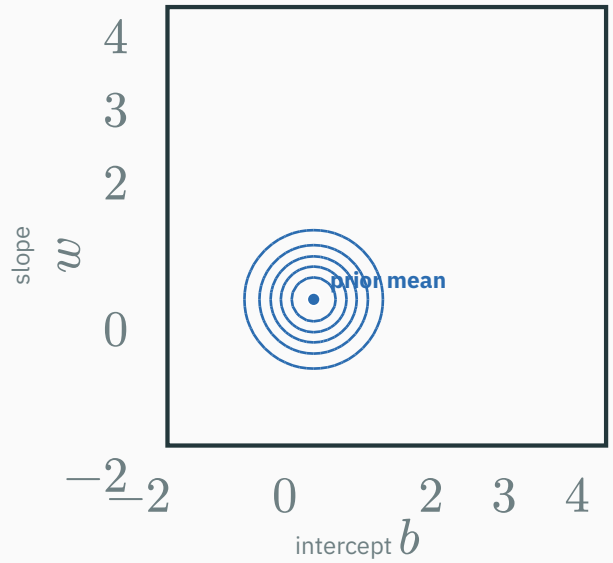

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The likelihood says “fit these data”; the prior says “prefer smaller coefficients”.

Bayes combines the regression likelihood and prior

$$p(b, w \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid b, w)\, p(b, w)}{p(\mathcal{D})}$$

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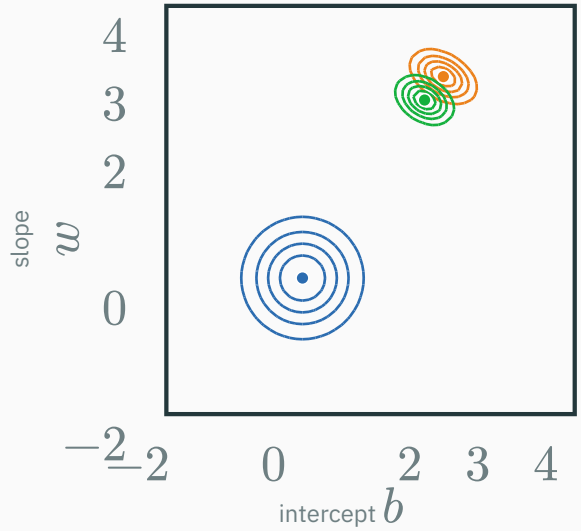


Contours: prior likelihood posterior

MLE $(2.07, 2.96)$ posterior peak $(1.79, 2.62)$ prior mean $(0, 0)$

The narrower prior visibly pulls the posterior peak away from the MLE and toward zero.

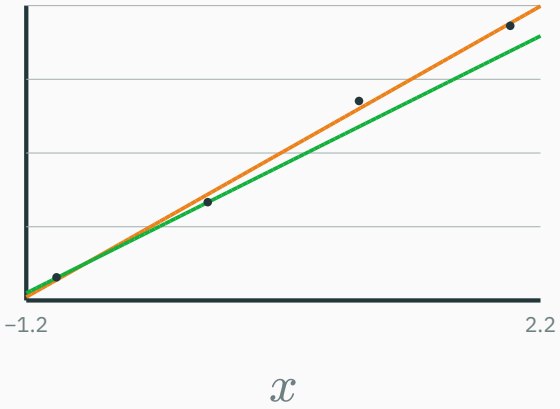
The prior changes the fitted line

V VISUAL

MLE, dashed MAP, solid

Moderate prior: $\tau = 0.5$

MAP: $\hat{y} = 1.79 + 2.62x$



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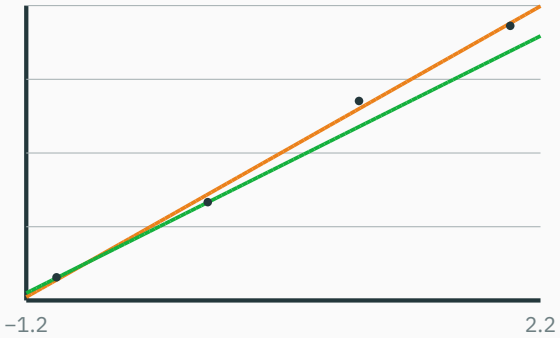
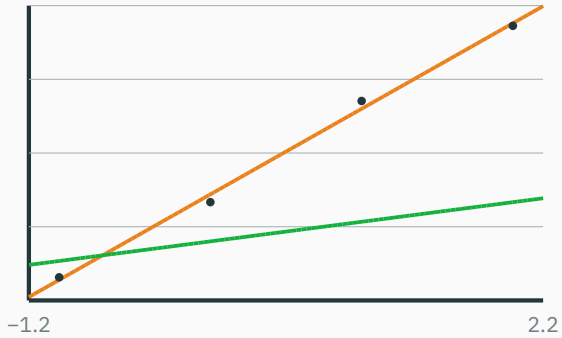


Much stronger prior: $\tau = 0.1$

MAP: $\hat{y} = 0.44 + 0.68x$



$$(b, w): \quad (2.07, 2.96)_{\text{MLE}} \rightarrow (1.79, 2.62)_{\text{moderate}} \rightarrow (0.44, 0.68)_{\text{strong}}$$

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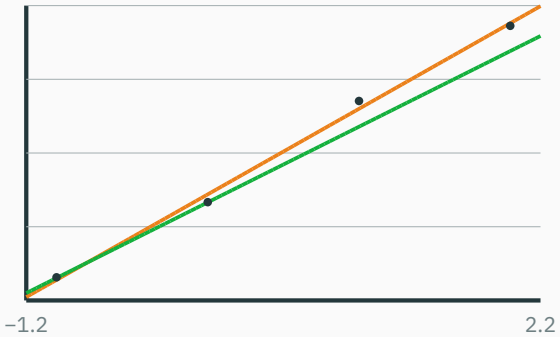

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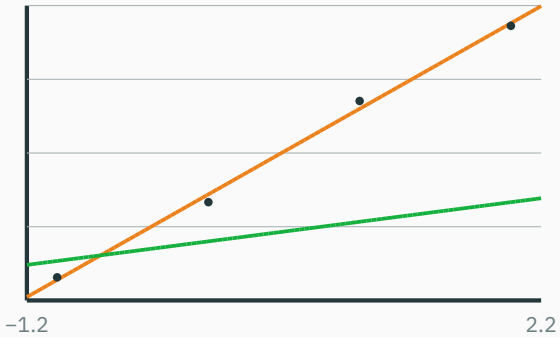

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Reducing τ puts more prior mass near the origin and moves both MAP coefficients much closer to zero.

A Gaussian prior is L_2 regularization

D DERIVATION

Assume the parameters are centred at zero before seeing the data:

$$\boldsymbol{\theta} \sim \mathcal{N}(\mathbf{0}, \tau^2 \boldsymbol{I}).$$

$$\underbrace{-\log p(\mathcal{D} \mid \boldsymbol{\theta})}_{\text{NLL}} + \underbrace{-\log p(\boldsymbol{\theta})}_{\text{negative log-prior}}$$

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$$\Rightarrow \quad \mathcal{L}_{\text{MAP}} = \text{NLL} + \underbrace{\frac{1}{2\tau^2}}_{\lambda} \|\boldsymbol{\theta}\|_2^2 + C$$

$\lambda = \frac{1}{2\tau^2}$: smaller $\tau \to$ larger $\lambda \to$ stronger shrinkage toward 0.

Gaussian MAP gives ridge shrinkage, step by step

D DERIVATION

For one coefficient, let $z = \hat{\theta}_{\mathrm{MLE}}$ be the likelihood centre and s its width:

$$p(\mathcal{D}|\theta) \propto \exp\!\left(-\tfrac{(\theta - z)^2}{2s^2}\right), \quad p(\theta) \propto \exp\!\left(-\tfrac{\theta^2}{2\tau^2}\right).$$

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$$\hat{\theta}_{\mathrm{MAP}} = \alpha z, \quad \alpha = \tfrac{\tau^2}{\tau^2+s^2} \in (0,1).$$

If $z = 0.6$ and $s = \tau$, then $\alpha = \frac{1}{2}$ and MAP $= 0.3$. Ridge reaches exactly zero only when $z = 0$.

Prior width controls how far MAP moves

V VISUAL

Same likelihood: $L(\theta) \propto \mathcal{N}\left(\theta; \hat{\theta}_{\text{MLE}} = 2, s^2\right)$ with $s = 0.6$; prior: $p(\theta) = \mathcal{N}(0, \tau^2)$.

$\hat{\theta}_{\text{MAP}} = \frac{\tau^2}{\tau^2 + s^2} \hat{\theta}_{\text{MLE}}$ (a shrinkage factor between 0 and 1)

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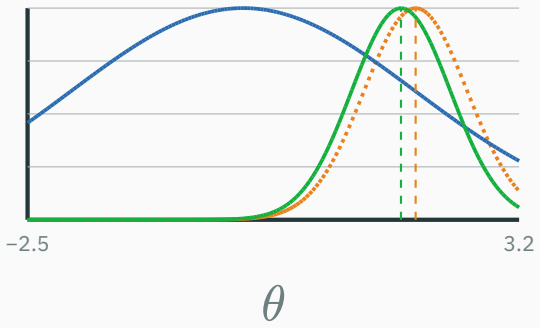
Broad prior: $\tau = 2, \lambda = 0.125$

$\text{MLE} = 2 \rightarrow \text{MAP} \approx 1.83$



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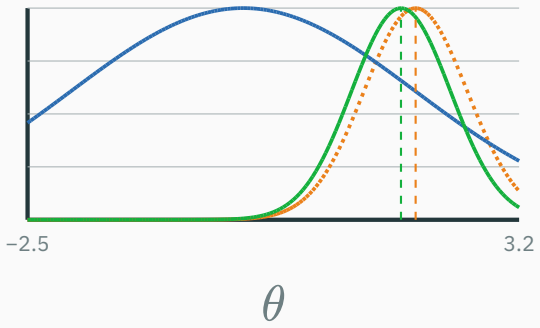
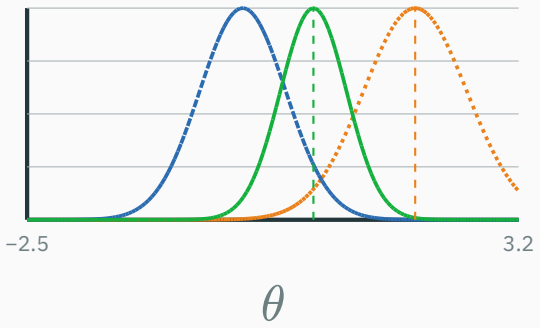


Narrow prior: $\tau = 0.5, \lambda = 2$

$\text{MLE} = 2 \rightarrow \text{MAP} \approx 0.82$



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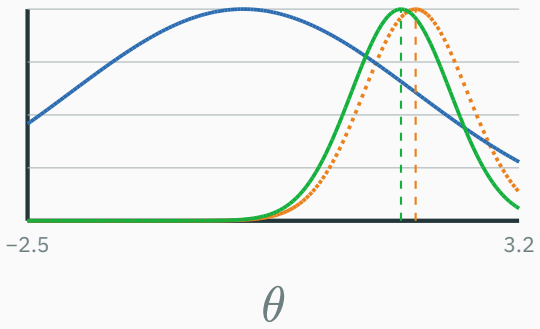

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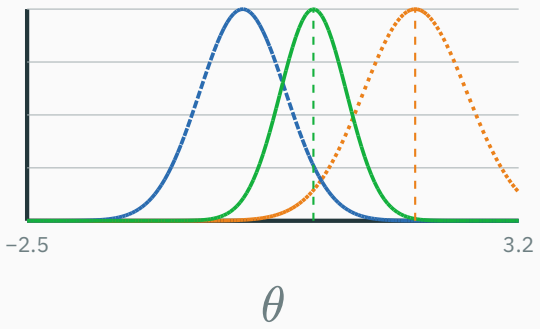

The narrower prior gives the larger λ and pulls MAP farther from the MLE toward zero.

A multivariate Gaussian prior has geometry

V VISUAL

$$\boldsymbol{\theta} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \quad -\log p(\boldsymbol{\theta}) = \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{\theta} - \boldsymbol{\mu}) + C$$

$\boldsymbol{\Sigma}$ is the covariance matrix; $\boldsymbol{\Sigma}^{-1}$ is the precision matrix, which determines how strongly each direction is penalized.

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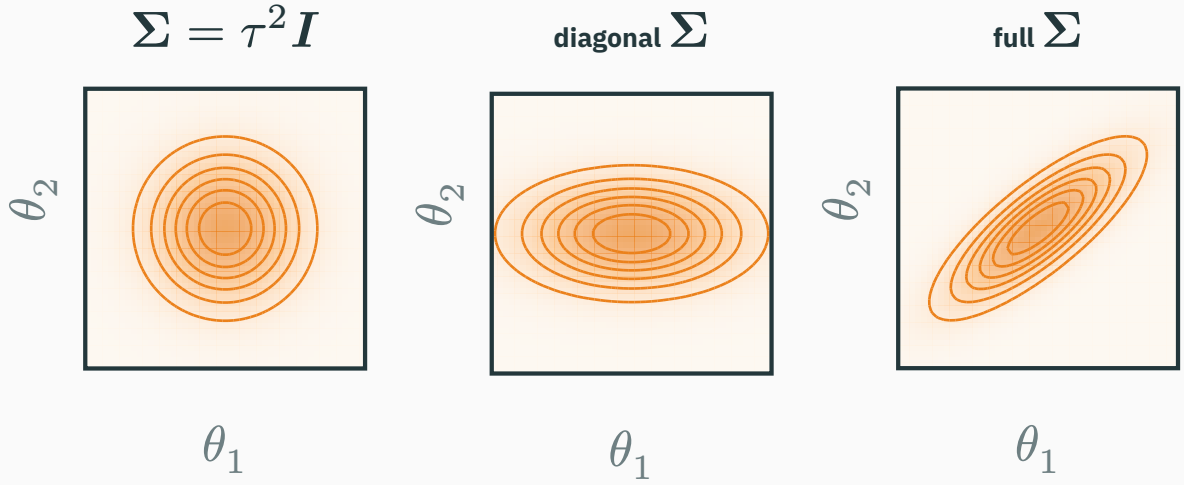

Axes: θ_1 and θ_2 are two coordinates of the parameter vector $\boldsymbol{\theta}$.

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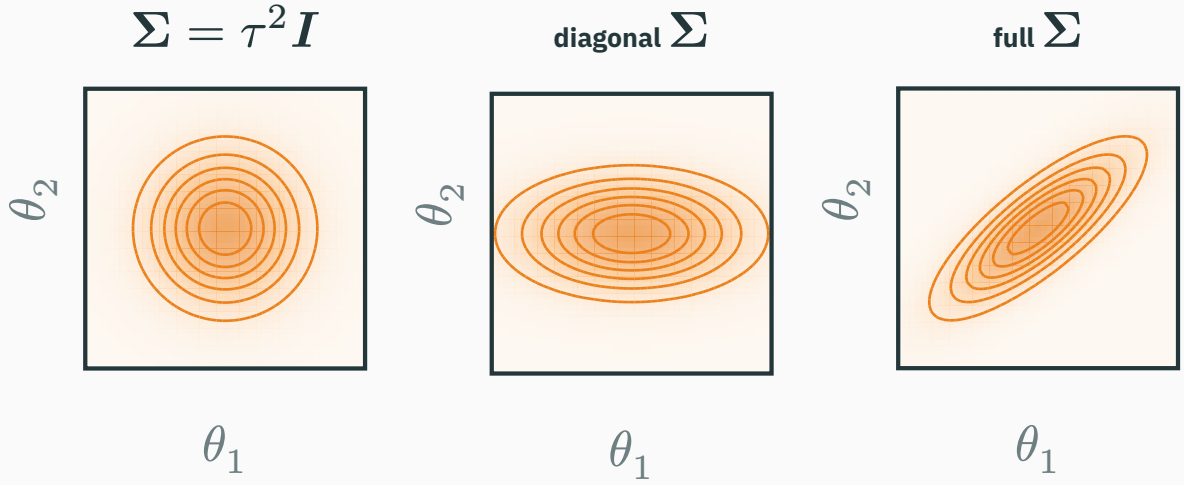

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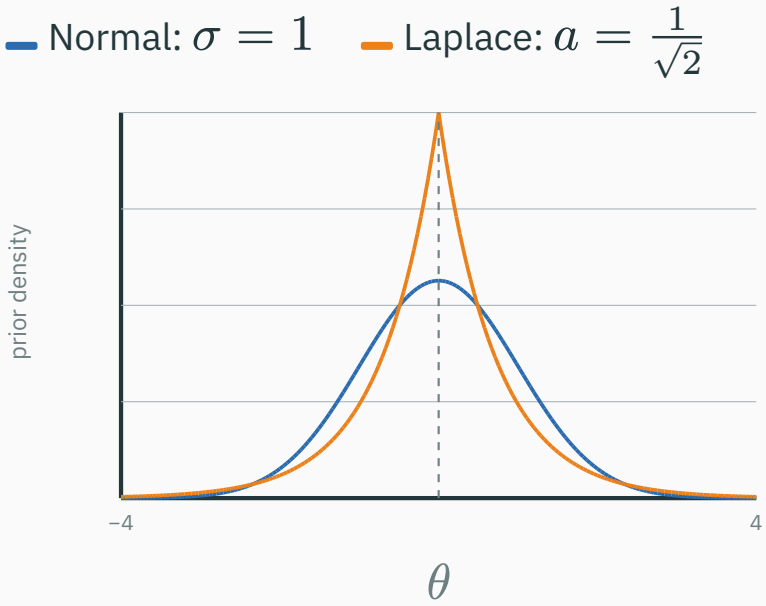
Covariance says **which directions in parameter space are plausible.**

Laplace is sharper at zero than a Normal prior

V VISUAL

Compare zero-centred priors with the **same variance**, 1:



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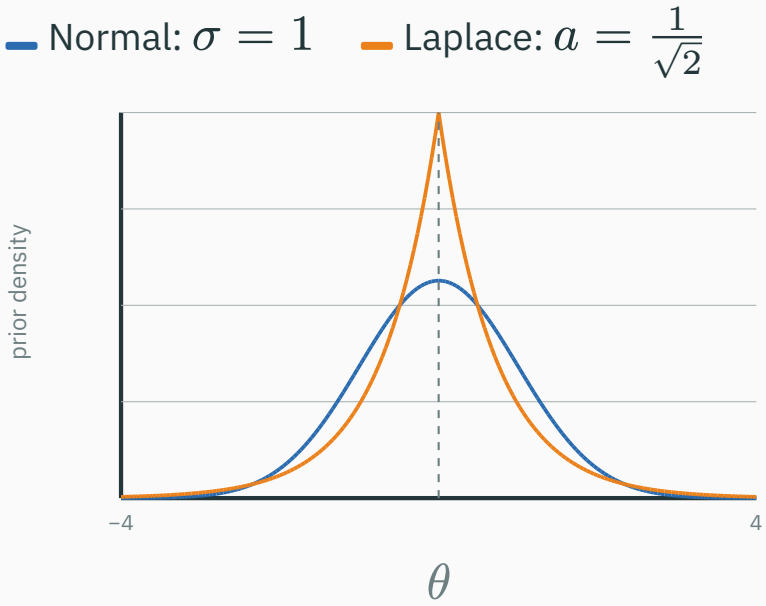

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- smooth around $\theta = 0$
- lighter tails

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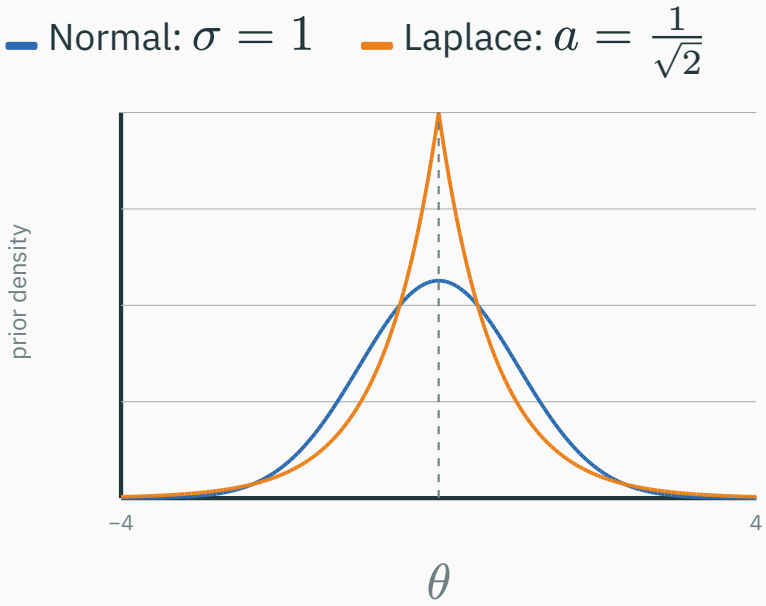

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The Laplace peak creates a corner in the negative log-prior. Next we derive why that corner can set coefficients exactly to zero.

Laplace MAP gives an L_1 objective

D DERIVATION

Use the scalar likelihood centred at $z = \hat{\theta}_{\mathrm{MLE}}$ and a zero-centred Laplace prior with scale a:

$$p(\mathcal{D}|\theta) \propto e^{-\frac{(\theta - z)^2}{2s^2}}, \quad p(\theta) = \frac{1}{2a} e^{-\frac{|\theta|}{a}}.$$

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For vectors, $\|\boldsymbol{\theta}\|_1 = \sum_j |\theta_j|$. Multiply by s^2; the minimizer does not change:

$$\tilde{J}_1(\theta) = \tfrac{1}{2}(\theta - z)^2 + \lambda|\theta|, \quad \lambda = \tfrac{s^2}{a}.$$

The Laplace negative log-prior is proportional to $|\theta|$, so MAP becomes an L_1-regularized optimization problem.

Soft thresholding follows from three cases

D DERIVATION

Differentiate $\tilde{J}_1(\theta) = \frac{1}{2}(\theta - z)^2 + \lambda|\theta|$ on either side of the corner.

Case 1: $\theta > 0$

$\tilde{J}_{1'} = \theta - z + \lambda$

$0 = \theta - z + \lambda$

$\theta = z - \lambda$, valid if $z > \lambda$

Case 2: $\theta < 0$

$\tilde{J}_{1'} = \theta - z - \lambda$

$0 = \theta - z - \lambda$

$\theta = z + \lambda$, valid if $z < -\lambda$

Case 3: $\theta = 0$

$\partial|\theta||_0 = [-1, 1]$

$0 \in -z + \lambda[-1, 1]$

valid iff $|z| \leq \lambda$

Soft thresholding follows from three cases

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$\tilde{J}_{1'} = \theta - z - \lambda$

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$\theta = z + \lambda$, valid if $z < -\lambda$

Case 3: $\theta = 0$

$\partial|\theta||_0 = [-1, 1]$

$0 \in -z + \lambda[-1, 1]$

valid iff $|z| \leq \lambda$

$$z > \lambda \quad \hat{\theta}_{\text{MAP}} = z - \lambda \qquad |z| \leq \lambda \quad \hat{\theta}_{\text{MAP}} = 0 \qquad z < -\lambda \quad \hat{\theta}_{\text{MAP}} = z + \lambda$$

$$\hat{\theta}_{\text{MAP}} = \text{sign}(z)\max(|z| - \lambda, 0).$$

Values inside the threshold band $[-\lambda, \lambda]$ map exactly to zero; values outside are pulled toward zero by λ.

Ridge shrinks; L_1 can threshold to exactly zero

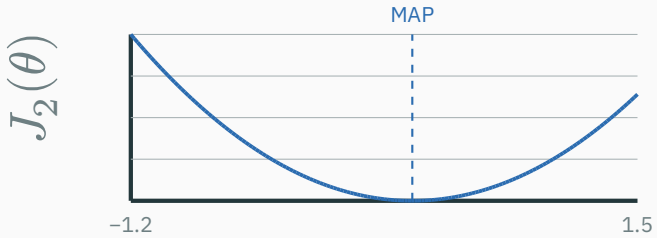
D DERIVATION

For one coefficient, let the data term be $D(\theta) = \frac{1}{2}(\theta - 0.6)^2$, centred at $z = 0.6$.

Normal prior $\rightarrow L_2$

$$J_2(\theta) = D(\theta) + \tfrac{1}{2}\theta^2$$

$$\hat{\theta}_{\text{MAP}} = \tfrac{z}{1+1} = 0.3$$



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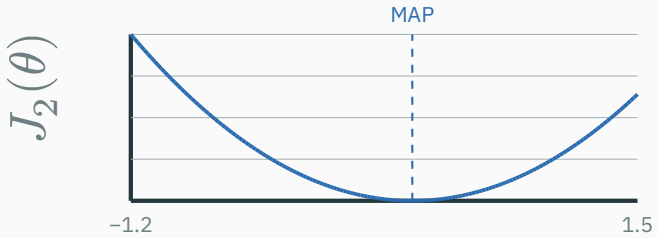

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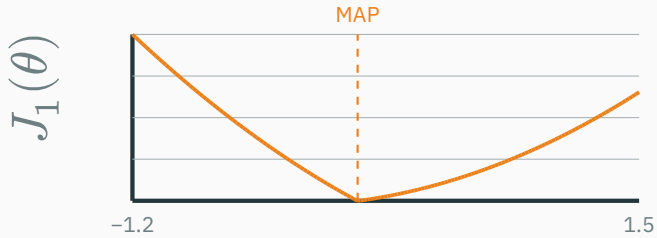

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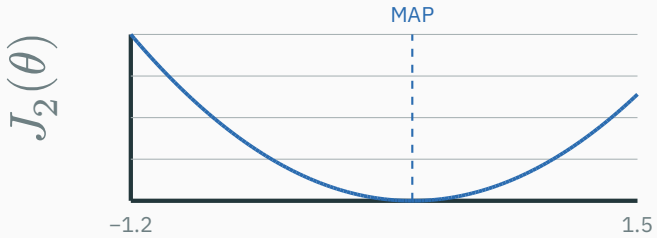

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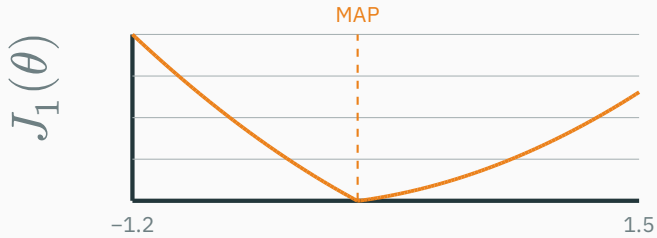
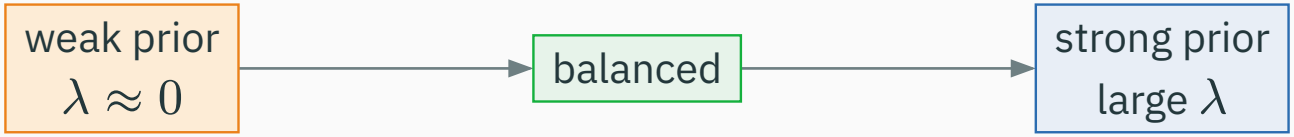


When the quadratic data term separates by coefficient—as with orthogonal features—L_1 applies this threshold coordinate by coordinate and can produce sparsity: many exact zeros.

Prior strength controls underfitting and overfitting

V VISUAL

For the summed-NLL convention used above, $\lambda = \frac{1}{2\tau^2}$:



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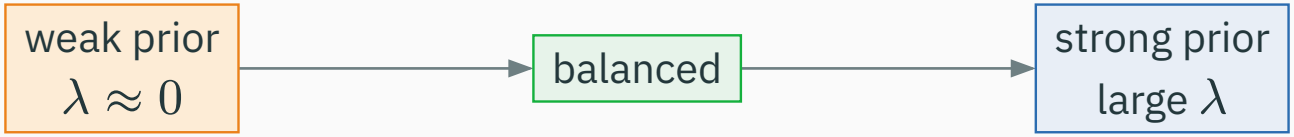

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flexible model

sensitive to this sample · overfit

LIKELIHOOD + PRIOR

enough flexibility

better generalization

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weights forced small

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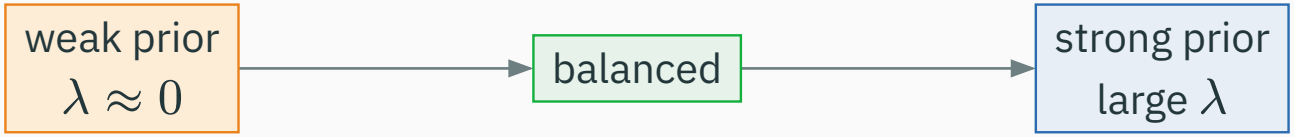

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Regularization trades flexibility for stability; more is not always better.

Interactive: likelihood, prior, MAP

I INTERACTIVE

INTERACTIVE

↗ nipunbatra.github.io/interactive-articles/map-regularization

map-regularization.html — a two-parameter linear model so contours are visible. Shows **likelihood**, **prior**, and **posterior** contours with the **MLE**, **MAP**, and zero points.
Controls: amount of data · noise · prior variance · Gaussian vs Laplace · prior correlation.

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Ask: more data? narrower prior? why does MAP → MLE as data grows? a correlated prior?

Full Bayes and deep learning

MAP is still one parameter vector

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Full Bayes keeps the whole posterior $p(\boldsymbol{\theta} \mid \mathcal{D})$ — a **distribution**, not a point.

Posterior predictive distribution

$$p(y^\star \mid \boldsymbol{x}^\star, \mathcal{D}) = \int p_{\boldsymbol{\theta}}(y^\star \mid \boldsymbol{x}^\star)\, p(\boldsymbol{\theta} \mid \mathcal{D})\, \mathrm{d}\boldsymbol{\theta}$$

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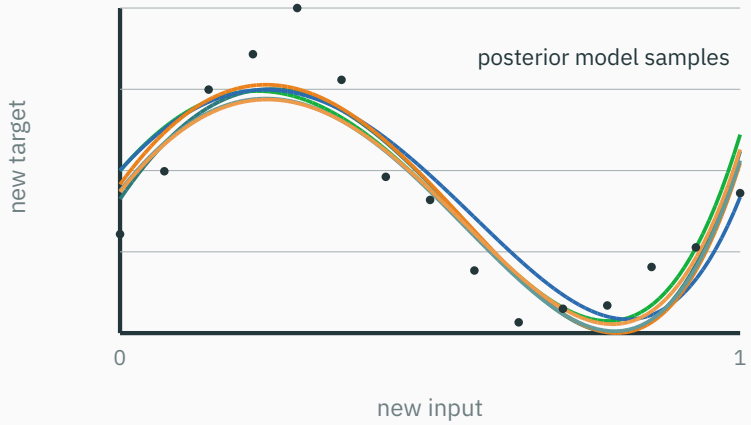

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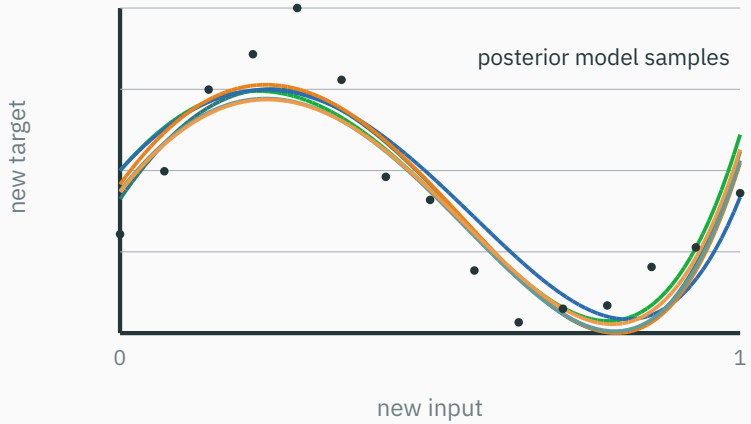

Bayesian prediction **averages over plausible models** — and reports uncertainty.

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A modern network has millions to billions of parameters, so integrating $p(\boldsymbol{\theta} \mid \mathcal{D})$ is hard.

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- MLE · MAP
- deep **ensembles**
- **dropout**-based approximations
- **variational inference**: fit a tractable approximate posterior

The standard supervised DL objective

B is the current minibatch; $|B|$ is its number of examples.

$$\min_{\boldsymbol{\theta}} \underbrace{\frac{1}{|B|} \sum_{i \in B} -\log p_{\boldsymbol{\theta}}(y_i \mid \boldsymbol{x}_i)}_{\text{likelihood / data fit}} + \underbrace{\lambda \|\boldsymbol{\theta}\|_2^2}_{\text{prior / regularization}}$$

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DL doesn't discard probabilistic ML — it **scales** it with expressive functions and gradient descent.

Retrieval summary

V VISUAL

Gaussian likelihood	$\Rightarrow$ **MSE**
Categorical likelihood	$\Rightarrow$ **cross-entropy**
Gaussian prior	$\Rightarrow L_2$
Laplace prior	$\Rightarrow L_1$
MLE + prior	$\Rightarrow$ **MAP**

Every supervised objective begins with two assumptions

V VISUAL

MODEL

observation model

$$p_{\boldsymbol{\theta}}(y \mid \boldsymbol{x})$$

parameter prior

$$p(\boldsymbol{\theta})$$

$\rightarrow$

TRAIN

$$\mathcal{L}_{\mathrm{MAP}}(\boldsymbol{\theta}) = \underbrace{\mathrm{NLL}(\mathcal{D}; \boldsymbol{\theta})}_{\text{data term}} + \underbrace{\Omega(\boldsymbol{\theta})}_{\text{parameter term}}$$

$$\Omega(\boldsymbol{\theta}) = -\log p(\boldsymbol{\theta})$$

$$\hat{\boldsymbol{\theta}}_{\mathrm{MAP}} = \arg\min_{\boldsymbol{\theta}} \mathcal{L}_{\mathrm{MAP}}$$

$\rightarrow$

PREDICT

plug-in: fix $\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}$

$$p_{\hat{\boldsymbol{\theta}}}(y^\star \mid \boldsymbol{x}^\star)$$

or average over the posterior

$$p(y^\star \mid \boldsymbol{x}^\star, \mathcal{D})$$

Loss $\leftrightarrow$ likelihood; regularizer $\leftrightarrow$ prior; prediction $\leftrightarrow$ plug-in or posterior predictive.

Next: from linear models to neural networks — **neurons, nonlinearities, and multilayer perceptrons.**