# Reading Group: An Introduction to PAC-Bayes

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# Introduction to PAC Generalisation Bounds

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**Please ask questions!**

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In the PAC setting, we view the learning algorithm as choosing a **hypothesis/predictor** $h \in \mathcal{H}$.

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- However, we don't know $D$, so we cannot compute $R(h)$.

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PAC bounds upper bound true risk $R(h_S)$ in terms of the empirical risk.

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Hence all randomness comes from sampling $S$:

- $S, h_S, r_S(h_S), R(h_S)$ are all random variables through $S$.
- $D$ is not random. $R(h)$ is non-random if $h$ is non-random (in particular, independent of $S$).

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- PAC bounds constitute a **worst-case analysis**.
- However, very weak assumptions! Typically just i.i.d. assumptions.
- No need to worry about priors or model mismatch!

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Want to bound the difference between true and empirical risk.

$$R(h) - r_S(h) = \mathbb{E}_{(x,y)\sim D}[\ell((x,y),h)] - \frac{1}{N}\sum_{(x,y)\in S}\ell((x,y),h)$$

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- **Concentration inequalities** bound deviations of this average.

# Hoeffding's Inequality

**Theorem 1 (Hoeffding).**

*Let $Z_1, \ldots, Z_N$ be i.i.d. random variables bounded in $[0, 1]$. Then for all $\epsilon > 0$,*

$$\mathbb{P}\left[\left|\frac{1}{N}\sum_{n=1}^{N} Z_n - \mathbb{E}[Z_n]\right| > \epsilon\right] \leq 2\exp(-2N\epsilon^2).$$

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Probability of a deviation greater than $\epsilon$ decreases as $\epsilon$ and $N$ increase.

By writing $\delta = 2\exp(-2N\epsilon^2)$, we get, with probability at least $1 - \delta$,

$$\left|\frac{1}{N}\sum_{n=1}^{N} Z_n - \mathbb{E}[Z_n]\right| \leq \sqrt{\frac{1}{2N}\log\frac{2}{\delta}}.$$

# A PAC Validation Bound

If we let $Z_n = \ell((x, y), h)$, Hoeffding's inequality immediately yields, with probability at least $1 - \delta$,

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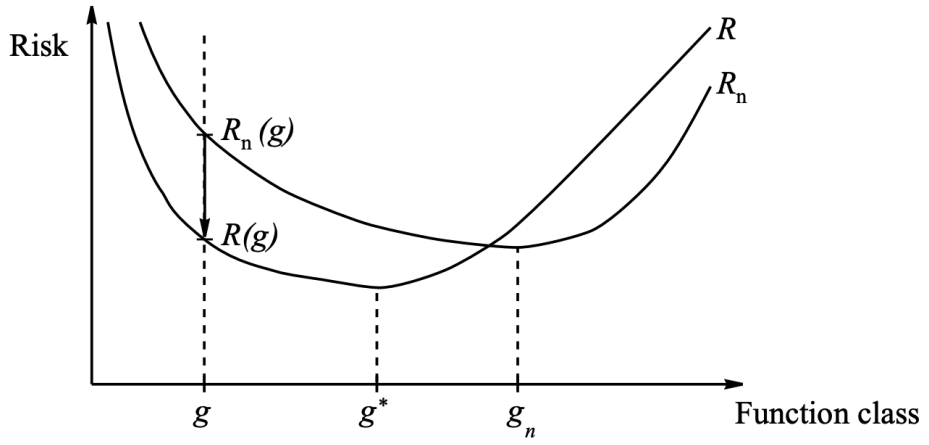


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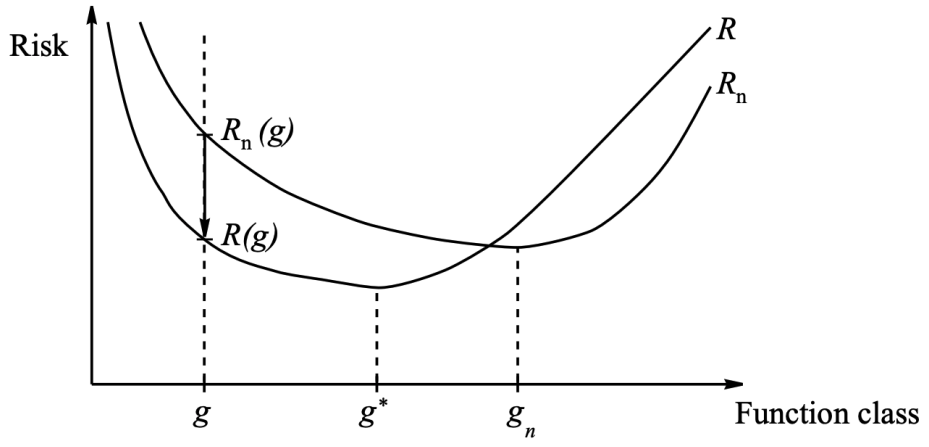


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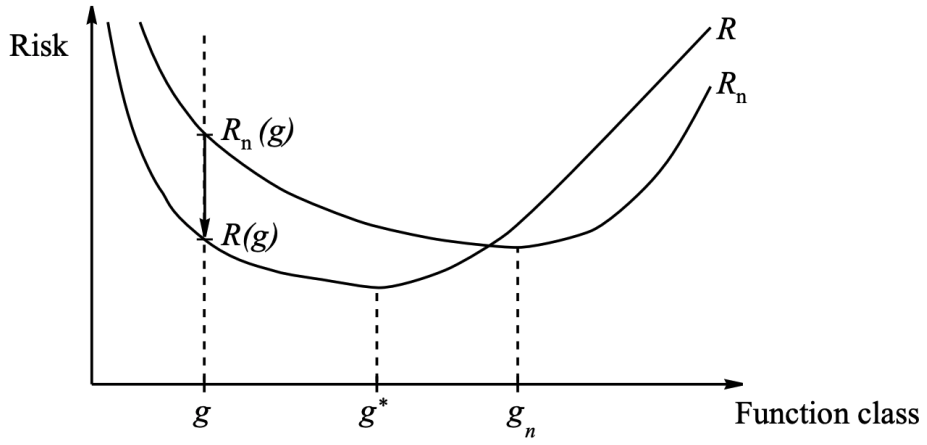


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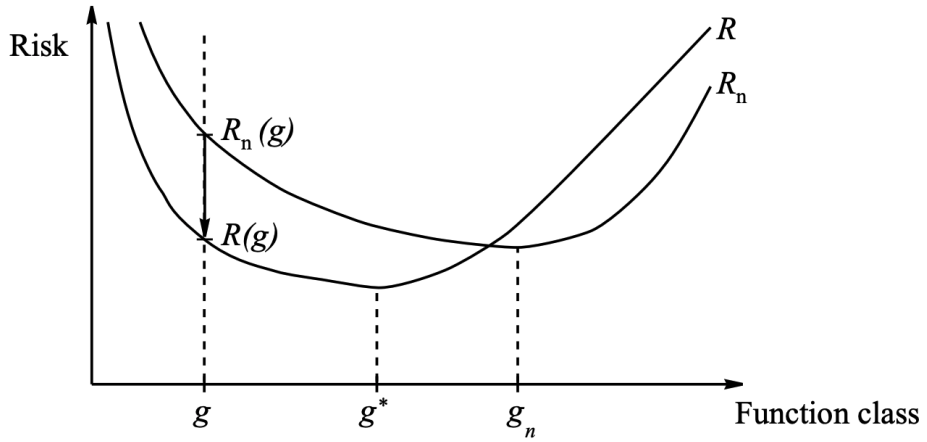


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- Switching order implies that with high probability, the curves $R_n$ and $R$ are close for all $g$ simultaneously!
- Latter statement more useful: allows us to *choose the hypothesis depending on S*.

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\begin{aligned}
&\mathbb{P}\left[\exists h \in \mathcal{H} : R(h) > r_S(h) + \sqrt{(2N)^{-1} \log(2/\delta)}\right] \\
&= \mathbb{P}\left[\bigcup_{h \in \mathcal{H}} \left\{S : R(h) > r_S(h) + \sqrt{(2N)^{-1} \log(2/\delta)}\right\}\right] \\
&\leq \sum_{h \in \mathcal{H}} \mathbb{P}\left[R(h) > r_S(h) + \sqrt{(2N)^{-1} \log(2/\delta)}\right] \\
&\leq |\mathcal{H}|\delta.
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- Identical to validation bound except for $\log|\mathcal{H}|$, which is a crude measure of "complexity".

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# PAC Bound for Finite Hypothesis Spaces

$$\mathbb{P}\left[\exists h \in \mathcal{H} : R(h) > r_S(h) + \sqrt{(2N)^{-1}\log(2/\delta)}\right] \leq |\mathcal{H}|\delta.$$

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- Yes — if we use *randomised* hypotheses, we can use PAC-Bayes!

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- **Warning:** The assumptions in PAC-Bayes are different than in Bayes.
  - Assumes data is i.i.d. from (unknown) distribution $D$,
  - No assumption that $P$ is related to a generating process/prior beliefs about the data.

# Mcallester's PAC-Bayes bound

**Theorem 2 (Mcallester's Theorem, McAllester, 1999, Maurer Variant).**

*For any $\ell \in \{0,1\}$, $D, \mathcal{H}$ and $P$ a probability measure supported on $\mathcal{H}$, for $N \geq 8$,*

$$R_Q \overset{1-\delta}{\leq} r_{S,Q} + \sqrt{\frac{\mathcal{D}_{\mathrm{KL}}\left[Q||P\right] + \log\sqrt{N} + \log\frac{2}{\delta}}{2N}} \tag{1}$$

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- If $\ell$ is the log-likelihood, minimizing this looks a lot like variational inference.
- Note if $|\mathcal{H}| < \infty$, $P$ is uniform and $Q$ is a point mass, then $\mathcal{D}_{\mathrm{KL}}\left[Q||P\right] = \log|\mathcal{H}|$, in which case this looks a lot like the union bound.

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**Lemma 3 (Change of Measure).**

$$\int \phi(h)q(h)d\lambda - \mathcal{D}_{\mathrm{KL}}\left[Q||P\right] = \log \int e^{\phi(h)}p(h)d\lambda - \mathcal{D}_{\mathrm{KL}}\left[Q||\hat{P}\right] \quad (2)$$

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- This is just the variational 'ELBO'!

# Proof of Change of Measure

We expand out the term $\mathcal{D}_{\mathrm{KL}}\left[Q||\hat{P}\right]$:

$$\int \log \frac{q(h)}{\hat{p}(h)} q(h) d\lambda = \int \log \frac{q(h)}{p(h)} \frac{p(h)}{\hat{p}(h)} q(h) d\lambda \tag{4}$$

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The second term on the RHS is,

$$\int \log \frac{\hat{p}(h)}{p(h)} q(h) d\lambda = \int \phi(h) q(h) d\lambda - \log \int e^{\phi}(h) p(h) d\lambda. \ \square$$

# Some Useful Inequalities

**Theorem 4 (Markov's inequality).**

*Let $X$ be a non-negative random variable. Then for any $a > 0$,* $\mathbb{P}(X > a\mathbb{E}[X]) < 1/a$.

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**Theorem 5 (Jensen's inequality).**

*Let $f$ be a convex function, and suppose $\mathbb{E}[X], \mathbb{E}[f(X)]$ are finite. Then*

$$f(\mathbb{E}[X]) \leq \mathbb{E}[f(X)].$$

# Proof of Mcallester's Bound

- Define $\Delta(R_Q, r_{S,Q}) = |R_Q - r_{S,Q}|^2$, our goal will be to upper bound $\Delta$ with high probability.

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# Finishing the Proof

It can be shown [Maurer, 2004] that,

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Putting this altogether,

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After rearranging gives,

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- There are also various generalizations e.g. that allow the prior to depend in certain ways on the data $S$ (e.g. Ambroladze et al. [2007]) or that allow for non-i.i.d. data (e.g. Ralaivola et al. [2009]).

# Applications to Neural Networks

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NNs can overfit but in practise don't: **why?**

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$$R(h) \leq r_S(h) + \sqrt{\frac{1}{2N}\left(\log|\mathcal{H}| + \log\frac{2}{\delta'}\right)}$$

With $\delta = 0.2$, we would need $N > 113,122$ for rhs to be $< 1$.
For ResNet50, $N > 255,078,163$.

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**Bounds are vacuous:** for empirically well-performing models on standard datasets, the generalisation error is bounded by a value greater than 1.

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**Hypothesis:** the complexity of functions found by fitting NN models is much lower than the number of network parameters would suggest.

# Nonvacous bounds for deep (stochastic) NN

Fix $\delta > 0$ and $P$ on $\mathcal{H}$. Collect dataset $s \sim D$. **Idea:** Optimise $Q$ with

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- Choose $P = \mathcal{N}(w;0,\lambda I)$. $\lambda$ is chosen from a predefined set using a union bound.

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- Local optima in flat regions have a smaller description length

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Intuition:

- Local optima in flat regions have a smaller description length
- This approach is very similar to Bayes by Backprop: we are approximately optimising a lower bound on the marginal likelihood.

# Nonvacous bounds for deep (stochastic) neural networks (some results)

| Experiment | T-600 | T-1200 | T-$300^2$ | T-$600^2$ | T-$1200^2$ | T-$600^3$ | R-600 |
|---|---|---|---|---|---|---|---|
| Train error | 0.001 | 0.002 | 0.000 | 0.000 | 0.000 | 0.000 | 0.007 |
| Test error | 0.018 | 0.018 | 0.015 | 0.016 | 0.015 | 0.013 | 0.508 |
| PAC-Bayes bound | 0.161 | 0.179 | 0.170 | 0.186 | 0.223 | 0.201 | 1.352 |
| KL divergence | 5144 | 5977 | 5791 | 6534 | 8558 | 7861 | 201131 |
| # parameters | 471k | 943k | 326k | 832k | 2384k | 1193k | 472k |
| VC dimension | 26m | 56m | 26m | 66m | 187m | 121m | 26m |

Table 1: Results for experiments on binary class variant of MNIST. SGD is either trained on (T) true labels or (R) random labels. The network architecture is expressed as $N^L$, indicating $L$ hidden layers with $N$ nodes each. Errors are classification error. The reported VC dimension is the best known upper bound (in millions) for ReLU networks. The SNN error rates are tight upper bounds (see text for details). The PAC-Bayes bounds upper bound the test error with probability $0.965$.

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- Bounds can warn us when our model will not generalise

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Zhou et al. [2019] leverage this interpretation to derive bounds for large networks after **pruning and quantization**.

On Imagenet, they obtain a bound of 96.5% while the validation error is 35%. (Non-vacuous!)

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Using Jensen's we can see:

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Here $\delta$ and $\psi_{P,D}(c,N) = \log \mathbb{E}_{h\sim P,\,(x,y)\sim D}[\exp(cN(R_h - r_{h,S}))]$, const. wrt. $Q$! If $c = 1$, this reduces to the ELBO.

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Minimising the above bound seems like it could be a good idea. Does the optima of $R_Q$ also minimise $CE_Q$?

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Otherwise we are learning under model misspecification.

# The Bayesian posterior is suboptimal under misspecification

Recall:

$$\underbrace{\mathbb{E}_{(x,y)\sim D}[-\log \mathbb{E}_{h\sim Q}[p(y|x,h)]}_{CE_Q} \leq \underbrace{\mathbb{E}_{h\sim Q}[\mathbb{E}_{(x,y)\sim D}[-\log p(y|x,h)]]}_{R_Q}$$

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This will only be a minimiser of $CE_Q$ if:

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for all $Q$. In other words: the single hypothesis $h^{\mathrm{ML}}$ is better than any model combination.

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$$H(D_{y|x}) = CE_{h^{\mathrm{ML}}}$$

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$$CE_Q \leq R_Q - V_Q \leq R_Q$$

where $V_Q$ is a variance encouraging term.

# Second order PAC-Bayes bounds

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$$\underbrace{\mathbb{E}_{(x,y)\sim D}[-\log \mathbb{E}_{h\sim Q}[p(y|x,h)]}_{CE_Q} \leq \underbrace{\mathbb{E}_{h\sim Q}[\mathbb{E}_{(x,y)\sim D}[-\log p(y|x,h)]]}_{R_Q}$$

We can sharpen our previous bound using a second order Jensen bound:

$$CE_Q \leq R_Q - V_Q \leq R_Q$$

where $V_Q$ is a variance encouraging term.

$$V_Q = \mathbb{E}_{(x,y)\sim D}[\frac{1}{\alpha(x,y)}\mathbb{E}_{h\sim Q}[\big(p(y|x,h) - \mathbb{E}_{h'\sim Q}p(y|x,h')\big)^2]]$$

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$V_Q$ takes positive values for posteriors different than a delta. It reduces to 0 otherwise (perfect model specification).

# Second order PAC-Bayes: Illustration

We can add this new term to our PAC-Bayes bound:

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$$CE_Q \leq R_Q - V_Q \leq r_{S,Q} - V_Q + \frac{\mathcal{D}_{\mathrm{KL}}\left[Q||P\right] - \log\delta + \psi_{P,D}(c,N)}{cN}$$

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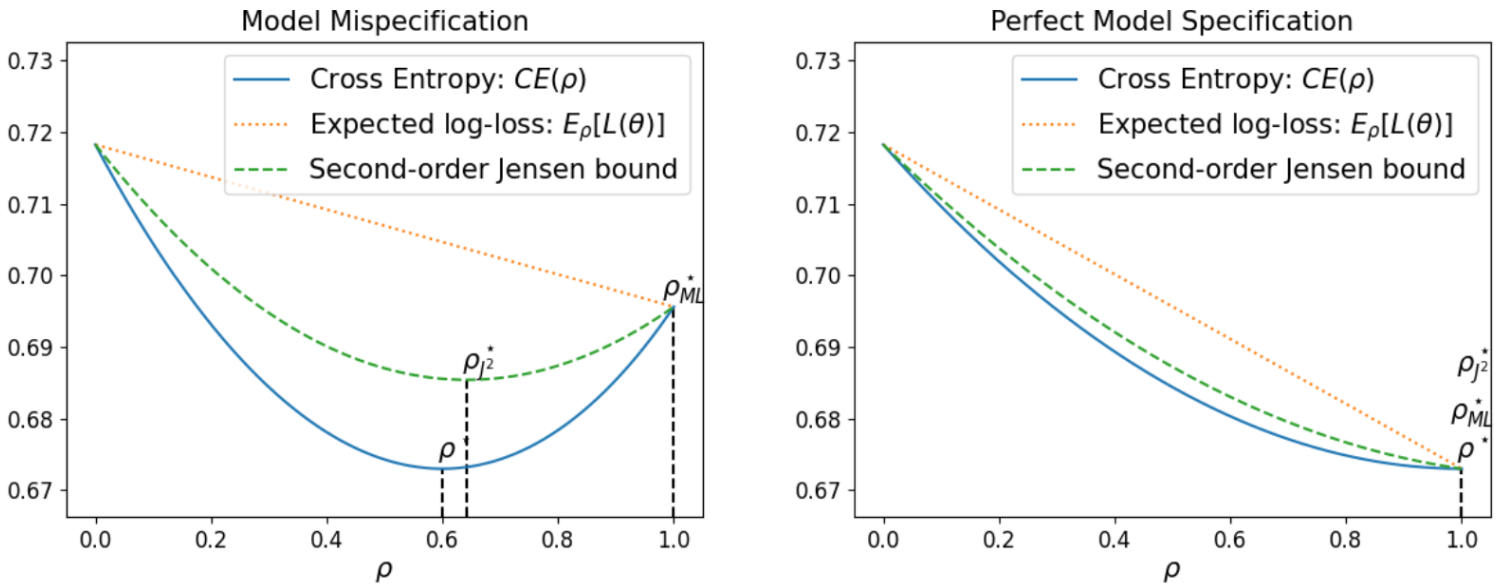


Figure 2: First-Order vs Second-Order Jensen Bounds. See Appendix B for full details.

# Second order PAC-Bayes: Misspecified noise model

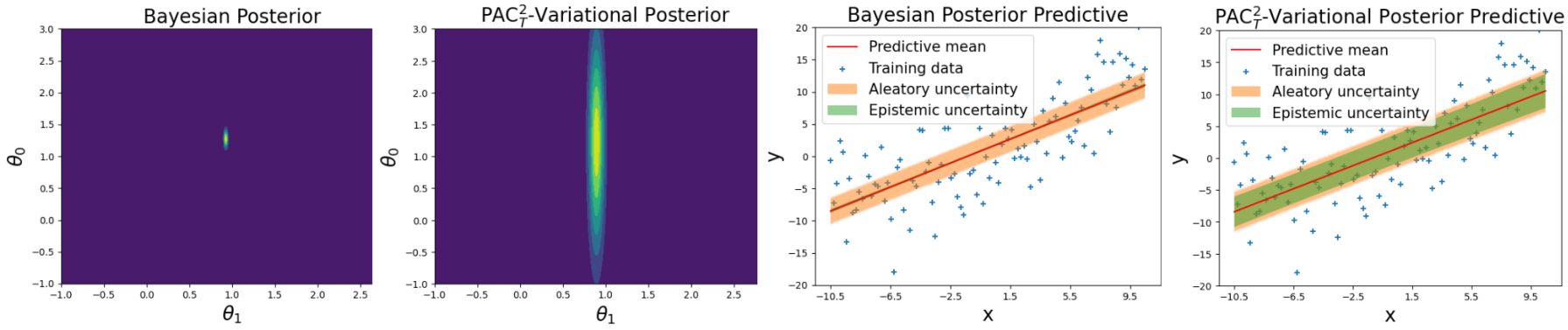


Figure 1: The exact Bayesian posterior and our new proposed (PAC$^2_T$-Variational) posterior, and their respective posterior predictive distributions, for a linear regression model with a misspecified constant noise term (the data noise is higher than the linear model's noise). The Bayesian posterior concentrates around the best single linear model, while our method estimates a posterior which introduces high variance in the intercept parameter $\theta_0$ to induce a posterior predictive distribution with higher noise that better fits the data distribution (see Appendix C.2 for details).

The new variance term is able to increase disagreement among hypothesis, increasing predictive variance.

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