Tutorial: Large Language Models and AI Agent Systems

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Outline

Part 1: Large Language Models

- What are LLMs
- Transformers
- Pre-Training & Fine-tuning
- Mainstream LLMs
- Capabilities & Limitations

Part 2: AI Agent

- Agent Architecture
- Reasoning
- RAG
- Tools & MCP

Part 3: Practices

- Toy LLM
- Toy MCP
- Toy Agent

Boom of Large Language Models

- **2017:** Transformer architecture introduced [1]
- **2018:** GPT-1, BERT [2]
- **2019–2020:** GPT-2, GPT-3 [3]
- **2022:** ChatGPT ignites the AI boom [4]
- **2023–2025:** GPT-4, Claude [5], Gemini [6], DeepSeek [7], Qwen [8], and other multimodal models.

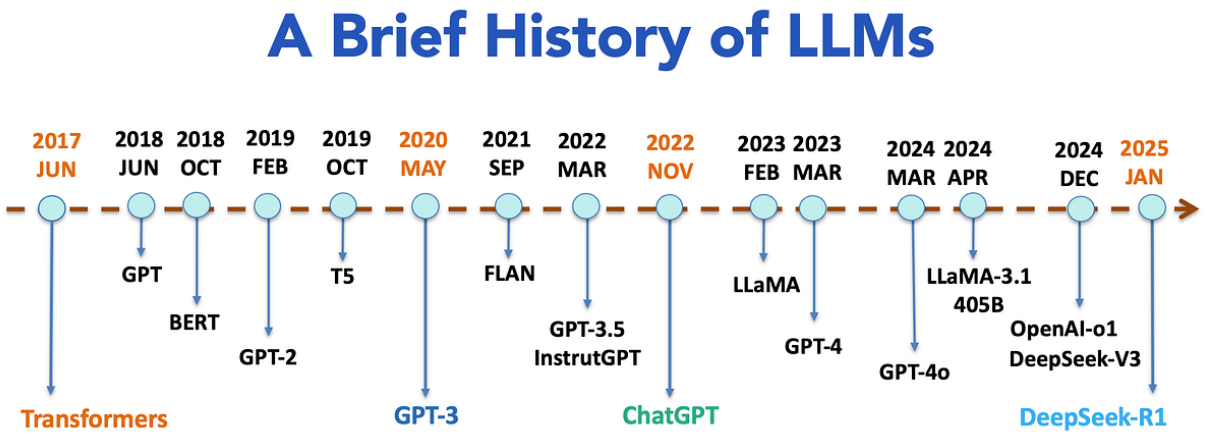


Figure: Timeline of notable LLM releases from Transformer (2017) to recent multimodal systems.

What are Large Language Models

Definition: Large Language Model

A Large Language Model (LLM) is a parameterized conditional probability model, mapping any finite token sequence (context) to a probability distribution over the next token in the vocabulary $\mathcal{V}$. The parameters θ are learned by maximizing log-likelihood over large-scale corpora [9].

$$f_\theta : \mathcal{V}^* \to \Delta(\mathcal{V}),$$

Mathematical Notation

- $\mathcal{V}$: token vocabulary (finite set of discrete symbols)
- $\mathcal{V}^*$: the set of all finite-length sequences over $\mathcal{V}$ (e.g., any prefix $w_{<t}$)
- $\Delta(\mathcal{V})$: the probability simplex over $\mathcal{V}$

$$\Delta(\mathcal{V}) = \{p : \mathcal{V} \to [0,1] \mid \sum_{v \in \mathcal{V}} p(v) = 1\}$$

- Induced joint distribution:

$$P_\theta(w_{1:n}) = \prod_{t=1}^{n} f_\theta(w_t \mid w_{<t})$$

Language Modeling

Language Modeling

Language modeling estimates the joint distribution over a sequence $w_{1:n} = (w_1, \ldots, w_n)$ by autoregressive factorization:

$$P_\theta(w_{1:n}) = \prod_{i=1}^{n} P_\theta(w_i \mid w_{<i}).$$

Training Objective

Maximum likelihood (cross-entropy minimization):

$$\mathcal{L}(\theta) = -\sum_{i=1}^{n} \log P_\theta(w_i \mid w_{<i}) \quad \Longleftrightarrow \quad \min_\theta \ \mathrm{CE}(P_{\text{data}}, P_\theta).$$

Language Modeling Metrics

- **Autoregressive generation:** The model predicts the next token given a prefix:

$$w_{t+1} \sim P_\theta(\cdot \mid w_{\leq t}),$$

- **Context window:** The model conditions only on the most recent L tokens:

$$P_\theta(w_t \mid w_{<t}) \approx P_\theta(w_t \mid w_{t-L:t-1}).$$

- **Perplexity (PPL):** For a sequence $w_{1:n}$, the average negative log-likelihood is

$$\mathcal{L}(\theta) = -\frac{1}{n} \sum_{t=1}^{n} \log P_\theta(w_t \mid w_{<t}).$$

  Perplexity is defined as:

$$\mathrm{PPL} = \exp\Big(\mathcal{L}(\theta)\Big) = \exp\left(-\frac{1}{n} \sum_{t=1}^{n} \log P_\theta(w_t \mid w_{<t})\right).$$

- **Interpretation:** Geometric mean of inverse probabilities. Lower is better.

$$\mathrm{PPL} = \left(\prod_{t=1}^{n} \frac{1}{P_\theta(w_t \mid w_{<t})}\right)^{\frac{1}{n}}.$$

Transformer Architecture

Core Innovation

Transformers replace recurrence with self-attention, enabling parallel token interactions and efficient modeling of long-range dependencies [1].

Layer Structure (Encoder/Decoder block) Given hidden states $H \in \mathbb{R}^{n \times d}$:

$$\tilde{H} = \mathrm{MHA}(H) + H, \qquad H^{+} = \mathrm{FFN}(\tilde{H}) + \tilde{H}.$$

Key Components

- **Self-attention** using learned projections (W_Q, W_K, W_V).
- **Multi-head attention** to attend in multiple subspaces.
- **Positional encoding** to inject sequence order.
- **Position-wise feed-forward network** for nonlinearity and mixing.
- **Residual connections + LayerNorm** for stable optimization.

Self-Attention Mechanism

Construction: For hidden states $H \in \mathbb{R}^{n \times d}$,

$$Q = HW_Q, \quad K = HW_K, \quad V = HW_V,$$

with projection matrices $W_Q, W_K, W_V \in \mathbb{R}^{d \times d}$. In multi-head attention, Q, K, V are reshaped into h heads.

Scaled Dot-Product Attention [1]

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}}\right) V.$$

Multi-Head Attention (MHA):

$$\text{MHA}(H) = \text{Concat}(\text{head}_1, \ldots, \text{head}_H) W_O.$$

Decoding Strategies in Large Language Models

Greedy Decoding

$$w_{t+1} = \arg\max_{w} P_\theta(w \mid w_{\leq t})$$

Deterministic but often repetitive.

Temperature Sampling Rescales logits before softmax:

$$P_T(w_i) = \frac{\exp(z_i/T)}{\sum_j \exp(z_j/T)}$$

$T < 1$: sharper; $T > 1$: more random.

Top-k Sampling Sample only from the k most probable tokens.

Top-p (Nucleus) Sampling Use smallest set V_p covering probability mass p [10]:

$$\sum_{i \in V_p} P(w_i) \geq p.$$

Adaptive truncation prevents tail degeneration.

Beam Search Maintains B candidate sequences:

$$\max_{w_{1:T}} \sum_{t=1}^{T} \log P_\theta(w_t \mid w_{<t})$$

Effective for translation; less suitable for open-ended chat.

Temperature: Effect on Softmax Distribution

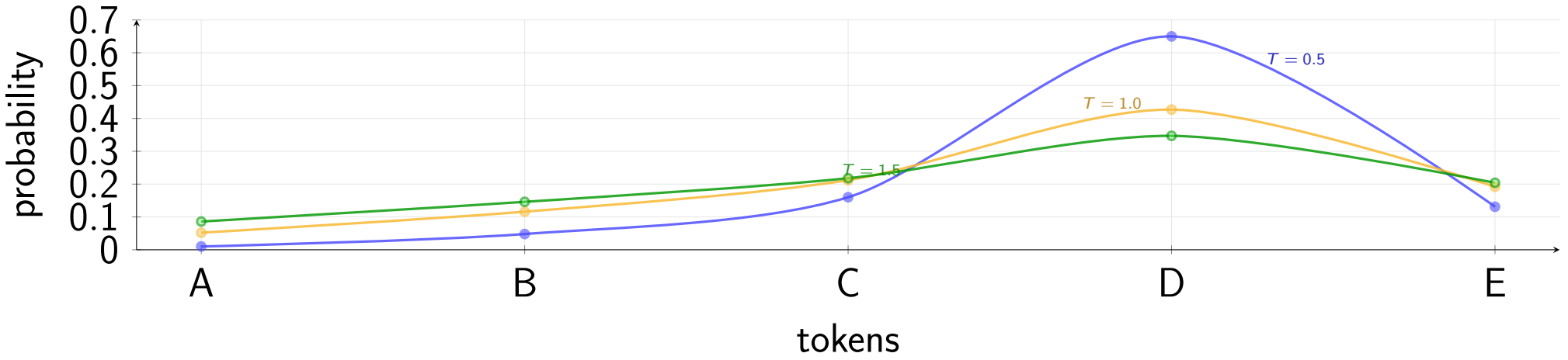
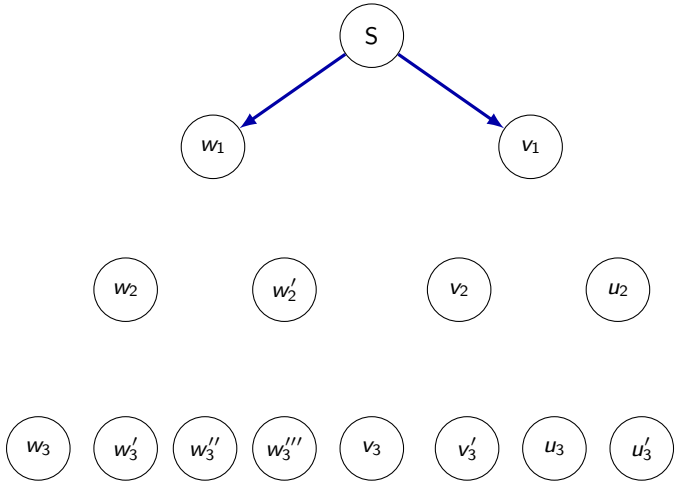


Figure: Temperature scaling reshapes the same logits.

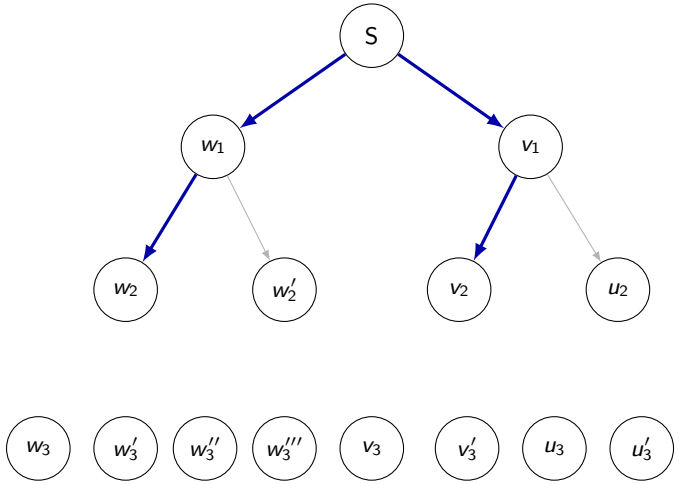
Beam Search (Beam Width $B = 2$)



Step 1: keep top-2 beams

Figure: Beam width $B = 2$: expand all candidates each step, keep the two highest-scoring prefixes (blue).

Beam Search (Beam Width $B = 2$)

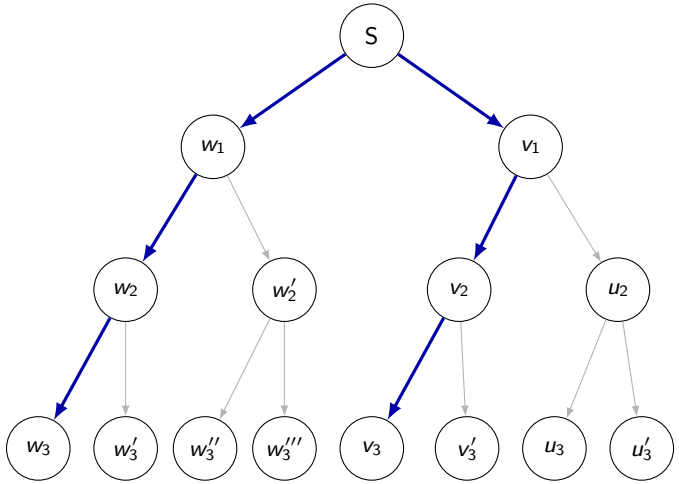


Step 1: keep top-2 beams

Step 2: re-score, keep new top-2

Figure: Beam width $B = 2$: expand all candidates each step, keep the two highest-scoring prefixes (blue).

Beam Search (Beam Width $B = 2$)



Step 1: keep top-2 beams

Step 2: re-score, keep new top-2

Step 3: repeat until stop

Figure: Beam width $B = 2$: expand all candidates each step, keep the two highest-scoring prefixes (blue).

Training Paradigm Evolution

From Pretraining to Alignment

- **Pretraining:** large-scale next-token prediction [3].

$$\min_{\theta} -\sum_{t} \log P_\theta(w_t \mid w_{<t})$$

  Foundation model learns general linguistic and world knowledge.

- **Fine-tuning (general concept):** adapt pretrained parameters θ_0 to a new distribution:

$$\theta^* = \arg\max_{\theta} \sum_{(x,y)\in\mathcal{D}_{ft}} \log P_\theta(y \mid x)$$

  Includes SFT, RLHF, RLAIF, DPO [11], etc.

Modern alignment pipeline:

$$\text{Pretraining} \rightarrow \text{SFT} \rightarrow \text{Preference Optimization (RLHF / RLAIF)}$$

Modern Alignment Techniques

Supervised Fine-Tuning (SFT)

- Dataset of instruction–response pairs $\mathcal{D}_{SFT} = \{(x_i, y_i)\}$.
- Optimize cross-entropy (teacher forcing) [4].
- Teaches format, compliance, basic helpfulness.

Reinforcement Learning from Human Feedback (RLHF)

- **Reward Model (RM)** trained on preference pairs [12].
- **PPO optimization** with KL constraint:

$$\max_{\theta} \mathbb{E}[\, r_\phi(x, y)\,] - \beta\, \mathrm{KL}(\pi_\theta \| \pi_{SFT})$$

- Improves helpfulness, harmlessness, and alignment.

RLAIF and Scalable Oversight

Reinforcement Learning from AI Feedback (RLAIF)

- Replace human preference labels with a strong AI judge.
- Construct AI preference pairs $(x, y^+, y^-)_{\text{AI}}$ [13].
- Enables scalable, cheaper, principle-based alignment (Constitutional AI).

Training Paradigm Summary

- **SFT**: learns to follow instructions.
- **RLHF**: aligns to human preferences.
- **RLAIF**: aligns via AI-based preference judgments.

$$\text{SFT: “can talk”} \quad \Rightarrow \quad \text{RLHF/RLAIF: “talks well”}$$

Major LLM Families

Decoder-Only Models (Autoregressive)

- GPT Series (OpenAI) [3]
- LLaMA (Meta) [14]
- Qwen (Alibaba) [8]
- Mistral / Mixtral (MoE) [15]
- DeepSeek [7]

Encoder-Only Models (Bidirectional)

- BERT (Google) [2]
- RoBERTa, ALBERT
- Focused on understanding tasks

Encoder–Decoder Models (Seq2Seq)

- T5 / FLAN-T5 [16]
- Strong for translation, summarization

Multimodal Models

- GPT-4 / GPT-4o (OpenAI)
- Gemini (Google) [6]
- Claude 3 (Anthropic) [5]

Notable Architectures and Innovations

Open-Source Ecosystem:

- **LLaMA**: flexible scales, strong baseline for fine-tuning.
- **Mistral/Mixtral**: efficient attention, MoE routing [15].
- **DeepSeek**: optimized training pipeline and inference efficiency [7].

Key Innovations:

- **MoE (Mixture of Experts):** Activates only a subset of parameters per token (Mistral, DeepSeek).
- **Long Context:** Handling 1M+ tokens (Gemini, Claude).
- **Attention Efficiency:** FlashAttention, RoPE, ALiBi.

Capabilities of Large Language Models

Core Strengths of LLMs [9]

- **Language Generation:** Produce coherent, context-aware text.
- **Semantic Understanding:** Encode rich contextual representations.
- **In-Context Learning:** Adapt to new tasks from examples without updates [3].
- **Reasoning Heuristics:** Chain-of-thought, code synthesis.
- **Multimodal Integration:** Align text, image, audio.
- **Knowledge Compression:** Store world knowledge in parameters.

LLMs are powerful *latent knowledge engines*.

Limitations & Motivation for AI Agents

Fundamental Limitations [17]

- **Lack of Groundedness:** No direct access to real-time information.
- **No Persistent Memory:** Context is bounded.
- **Unreliable Reasoning:** Hallucinations.
- **Static Knowledge:** Knowledge is "frozen" at training time.
- **Weak Action Capabilities:** Cannot execute actions reliably.

Why AI Agents?

- Integrate LLMs with **tools**, **memory**, **environment** [18].
- Enable planning, real-world actions, continual information gathering.
- Transform LLMs from passive text generators to **autonomous problem-solvers**.

What Are AI Agents?

Definition

An **AI Agent** is a system that uses an LLM as its core controller to **perceive**, **reason**, and **act** within an external environment [18]. Formally, an agent defines a policy

$$\pi : \mathcal{O}^* \to \mathcal{A},$$

mapping a history of observations $\mathcal{O}^*$ to actions $\mathcal{A}$ [17].

Key Characteristics

- **Autonomy:** Operates in iterative loops (The "Agentic Loop") without continuous human intervention.
- **Goal-driven:** Executes high-level objectives rather than just responding to prompts [19].
- **Tool Usage:** Interacts with external APIs (Search, Calculator, Code Interpreter).

Paradigm Shift: Copilot vs. Agent

Copilot (Human-in-the-loop)

- **Role:** Assistant / Draftsman.
- **Trigger:** User explicitly prompts every step.
- **Flow:** Linear (Input $\rightarrow$ Output).
- *Example:* GitHub Copilot, ChatGPT.

Agent (Human-on-the-loop)

- **Role:** Actor / Executor.
- **Trigger:** User sets a high-level goal.
- **Flow:** Looping (Thought $\rightarrow$ Action $\rightarrow$ Observation).
- *Example:* AutoGPT, Devin.

The Cognitive Architecture

An Agent is not just a model; it is a system designed to act autonomously. Based on Lilian Weng's architecture [18]:

Core Components:

1. **Brain (LLM):** The core controller for reasoning and planning.
2. **Memory:** Stores history and knowledge.
3. **Planning:** Task decomposition and self-reflection.
4. **Tools:** Executing actions and manipulating environments.

Memory Systems in Agents

Inspired by human cognitive science, Agent memory is categorized into three types [19]:

1. **Working Memory (Short-term):**
   - *Implementation:* The Context Window.
   - *Function:* Stores current reasoning steps, immediate observations, and scratchpad data.
2. **Episodic Memory (Experience):**
   - *Implementation:* Vector Database (Logs/Trace).
   - *Function:* Recalling past events, user interactions, and outcomes of previous actions to learn from experience.
3. **Semantic Memory (Knowledge):**
   - *Implementation:* Model Weights + RAG (Knowledge Base).
   - *Function:* Storing facts about the world (e.g., "The capital of France") independent of personal experience.

Reasoning: Beyond Simple Prompting

Agents require structured thinking to solve complex, multi-step problems.

- **Chain of Thought (CoT):** *"Let's think step by step."* Decomposing a problem into linear intermediate steps [20].
- **Tree of Thoughts (ToT):** Generalizes CoT by exploring multiple "branches" of reasoning possibilities. The agent can look ahead, backtrack, and evaluate different paths globally [21].
- **Reflexion (Self-Correction):** An architecture where the agent critiques its own past failures. It generates a "verbal reinforcement" trace to avoid repeating mistakes in the next attempt [22].

RAG: The Agent's Library

RAG bridges the gap between the frozen parametric knowledge of the LLM and dynamic external data [23].

Why Agents Need RAG?

- **Hallucination Reduction:** Grounds answers in retrieved documents.
- **Dynamic Knowledge:** Access to up-to-date information (e.g., stock prices, recent news) without retraining.
- **Domain Specificity:** Access to private enterprise data.

The Flow:

$$\text{Query} \xrightarrow{\text{Embed}} \text{Vector Search} \xrightarrow{\text{Retrieve}} \xrightarrow{\text{Augment Prompt}} \text{LLM}$$

Tools & Action Execution

Agents use tools to affect the world, turning text output into executable actions [24].

The Tool Execution Loop

1. **Select:** LLM decides which tool to call based on the prompt.
2. **Generate:** LLM formats valid JSON arguments (e.g., ‘”calc”: ”12*4”‘).
3. **Execute:** The runtime (Python/API) runs the function.
4. **Observe:** Result feeds back into Working Memory.

The Integration Challenge

Without a standard, connecting Agents to data is an $O(M \times N)$ problem.

- **The Silo Issue:** Developers must write specific integration code for every data source (Google Drive, Slack, GitHub) for every different Agent implementation [25].
- **Fragmentation:** An agent built for Claude Desktop cannot easily access tools built for a LangChain application.
- **Maintenance Nightmare:** API changes in a data source break all connected agents.

Enter MCP: The "USB-C" for AI

Model Context Protocol (MCP) is an open standard that unifies how AI models interact with data and tools [26].

Core Philosophy: "Build once, run anywhere."

MCP Architecture [27]

- **MCP Host:** The application where the AI model runs (e.g., Claude Desktop, IDEs like Cursor/Windsurf). It manages the connection lifecycle.
- **MCP Client:** The protocol implementation within the Host. It maintains 1:1 connections with Servers and handles permission negotiation.
- **MCP Server:** A lightweight bridge to a specific data source. It exposes capabilities (Resources, Tools) to the Client without knowing the implementation details of the Host.

MCP Primitives: What Servers Expose

MCP Servers expose three primary primitives to the Agent [27]:

1. **Resources (Passive Context):**
   - *Role:* Reading data (File content, database rows, logs).
   - *Analogy:* Like ‘GET‘ requests; providing the "ground truth".
2. **Tools (Active Capabilities):**
   - *Role:* Executing actions (API calls, scripts).
   - *Analogy:* Like ‘POST‘ requests; model-controlled execution.
3. **Prompts (Reusable Workflows):**
   - *Role:* Pre-defined templates to help users leverage the server.
   - *Example:* A "Debug Error" prompt that automatically loads the error log Resource and the code context.

Building AI Agent Systems

Hands-on focus

From a toy Transformer to a chat agent with tools and a runnable UI stack.

- **LLM build and pretrain** — craft a minimal Transformer in `torch`, wire a tiny dataset, and pretrain/inspect with `deepspeed`.
- **MCP server & client** — define resources and tools, ship prompts, and exercise them via a toy command-line client.
- **Agent workflow** — assemble a chat agent that hits the MCP tools, with a lightweight frontend, backend, and workflow engine.

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